10526940aa search claims 1-3

10526940species

=> fil stng
COST IN U.S. DOLLARS — SINCE FILE ENTRY: TOTAL SESSION

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.85	1166.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) — SINCE FILE ENTRY: TOTAL SESSION

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-62.40

FILE 'STNGUIDE' ENTERED AT 16:07:25 ON 01 MAR 2007
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Feb 23, 2007 (20070223/UP).

=> fil reg
COST IN U.S. DOLLARS — SINCE FILE ENTRY: TOTAL SESSION

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.84	1167.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) — SINCE FILE ENTRY: TOTAL SESSION

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-62.40

FILE 'REGISTRY' ENTERED AT 16:16:00 ON 01 MAR 2007
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1
DICTIONARY FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10526940notspec.str

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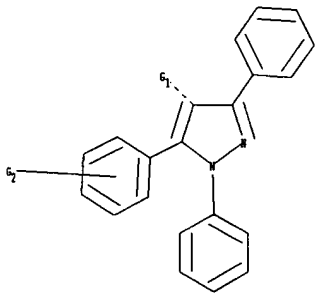

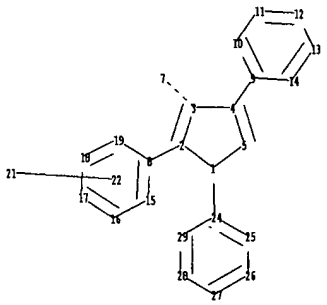

chain nodes :
7 21
ring nodes :
1 2 3 4 5 8 9 10 11 12 13 14 15 16 17 18 19 24 25 26 27 28 29

chain bonds :
1-24 2-8 3-7 4-9
ring bonds :
1-2 1-5 2-3 3-4 4-5 8-15 8-19 9-10 9-14 10-11 11-12 12-13 13-14 15-16
16-17 17-18 18-19 24-25 24-29 25-26 26-27 27-28 28-29
exact/norm bonds :
1-2 1-5 1-24 3-7 4-5
exact bonds :
2-3 2-8 3-4 4-9
normalized bonds :
8-15 8-19 9-10 9-14 10-11 11-12 12-13 13-14 15-16 16-17 17-18 18-19
24-25 24-29 25-26 26-27 27-28 28-29
isolated ring systems :
containing 1 : 8 : 9 :

G1:H,CH3

G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 21:CLASS
22:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom

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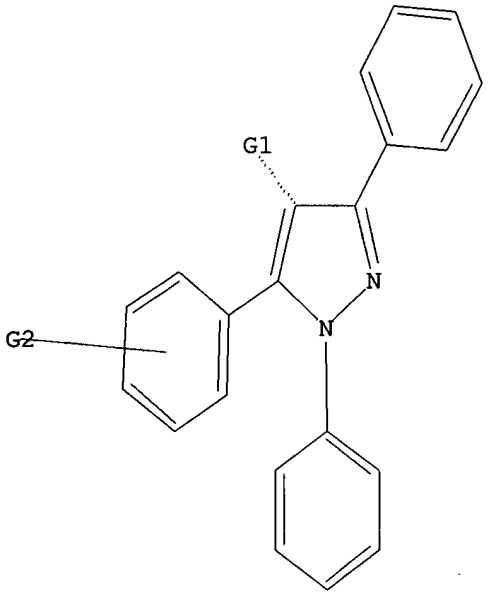
L23 STRUCTURE UPLOADED

=> d
L23 HAS NO ANSWERS
L23 STR



G1 H,Me
G2 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Structure attributes must be viewed using STN Express query preparation.

=> d his

(FILE 'HOME' ENTERED AT 15:24:30 ON 01 MAR 2007)

FILE 'REGISTRY' ENTERED AT 15:24:37 ON 01 MAR 2007
L1 STRUCTURE UPLOADED
L2 49 S L1
L3 11773 S L1 FULL
L4 STRUCTURE UPLOADED
L5 580 S L4 FULL SUB=L3

FILE 'CAPLUS' ENTERED AT 15:26:43 ON 01 MAR 2007
L6 470 S L5
L7 STRUCTURE UPLOADED
L8 2416251 S D

FILE 'REGISTRY' ENTERED AT 15:28:43 ON 01 MAR 2007
L9 0 S L7 SUB=L5 FULL
L10 0 S L7 FULL SUB=L3

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L14           55 S L13 FULL

     FILE 'CAPLUS' ENTERED AT 15:32:16 ON 01 MAR 2007
L15           27 S L14

     FILE 'REGISTRY' ENTERED AT 15:33:56 ON 01 MAR 2007
L16             STRUCTURE UPLOADED
L17         8423 S L16 FULL  SUB=L3

     FILE 'REGISTRY' ENTERED AT 15:50:55 ON 01 MAR 2007
L18             STRUCTURE UPLOADED
L19           38 S L18
L20         2044 S L18 FULL

     FILE 'CAPLUS' ENTERED AT 15:51:22 ON 01 MAR 2007
L21          111 S L20

     FILE 'STNGUIDE' ENTERED AT 15:52:00 ON 01 MAR 2007

     FILE 'REGISTRY' ENTERED AT 16:06:16 ON 01 MAR 2007
L22            1 S 178625-21-3/RN

     FILE 'STNGUIDE' ENTERED AT 16:07:25 ON 01 MAR 2007

     FILE 'REGISTRY' ENTERED AT 16:16:00 ON 01 MAR 2007
L23             STRUCTURE UPLOADED
L24         1636 S L23 FULL  SUB=L20

=> d l20 not l24
L24 IS NOT VALID HERE
For an explanation, enter "HELP DISPLAY".

=> s l20 not l24
L25         408 L20 NOT L24

=> fil caplus
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                              ENTRY    SESSION
FULL ESTIMATED COST                            44.70    1212.38

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                              ENTRY    SESSION
CA SUBSCRIBER PRICE                             0.00     -62.40

FILE 'CAPLUS' ENTERED AT 16:21:14 ON 01 MAR 2007
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FILE LAST UPDATED: 28 Feb 2007 (20070228/ED)

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=> s l25
L26 56 L25

=> d ibib abs hitstr tot

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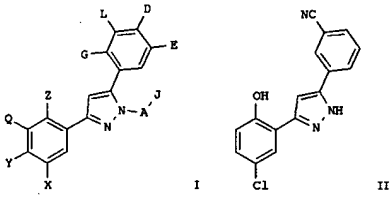
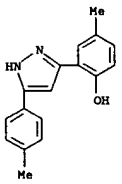
L26 ANSWER 1 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1095978 CAPLUS
DOCUMENT NUMBER: 145:438611
TITLE: Preparation of 3,5-diphenylpyrazoles as antitumor agents
INVENTOR(S): Kuroiwa, Shunsuke; Maruyama, Sakiko; Suzuki, Yoshikazu; Yamazaki, Hiroko
PATENT ASSIGNEE(S): Nippon Kayaku Kabushiki Kaisha, Japan
SOURCE: PCT Int. Appl., 45pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006109680	A1	20061019	WO 2006-JP307346	20060406
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

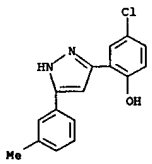
PRIORITY APPLN. INFO.: JP 2005-110717 A 20050407
OTHER SOURCE(S): MARPAT 145:438611
GI



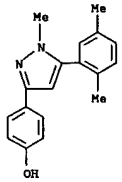
AB Title compds. I [wherein A = H, carbonyl or sulfonyl; J = (un)substituted alkyl or amino; G, Z = H, OH, alkoxy, etc.; D, E, L, Q, X, Y = H, (un)substituted aminocarbonyl, alkoxycarbonyl, etc., D and L, and Q and Y may link together to form a N/S-heterocyclyl ring, with limitations] and



RN 912967-83-0 CAPLUS
CN Phenol, 4-chloro-2-[5-(3-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



IT 362006-35-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(reference; preparation of diphenylpyrazoles as antitumor agents)
RN 362006-35-7 CAPLUS
CN Phenol, 4-[5-(2,5-dimethylphenyl)-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS

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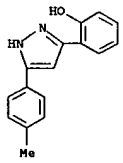
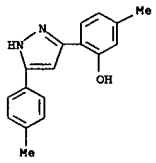
pharmaceutically acceptable salts thereof were prepd. as anticancer agents. For instance, treatment of 5'-chloro-2'-hydroxyacetophenone with 3-cyanobenzoyl chloride followed by cyclization with hydrazine hydrate gave diphenylpyrazole II. This product showed cell growth inhibition with IC50 of 0.23 μg/mL against MCF-7 cells and 0.066 μg/mL against MDA-MB-453 cells, resp. Therefore, the invented compds. and their pharmaceutical compns. are useful for the treatment of various cancer, such as breast cancer and lung cancer.

IT 384352-30-1P 416877-12-8P 416880-94-9P
912967-83-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of diphenylpyrazoles as antitumor agents)
RN 384352-30-1 CAPLUS
CN Phenol, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 416877-12-8 CAPLUS
CN Phenol, 5-methyl-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

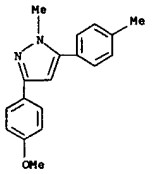


RN 416880-94-9 CAPLUS
CN Phenol, 4-methyl-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

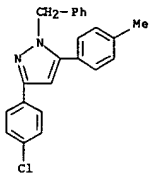
10526940species

L26 ANSWER 2 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:660707 CAPLUS
DOCUMENT NUMBER: 145:292939
TITLE: Reaction of N-Monosubstituted Hydrazones with Nitroolefins: A Novel Regioselective Pyrazole Synthesis
AUTHOR(S): Deng, Xiaohu; Mani, Neelakandha S.
CORPORATE SOURCE: Department of Drug Discovery, Johnson & Johnson Pharmaceutical R & D LLC, San Diego, CA, 92121, USA
SOURCE: Organic Letters (2006), 8(16), 3505-3508
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A novel regioselective synthesis of substituted pyrazoles from N-monosubstituted hydrazones and nitroolefins is described. The reaction is performed in a one-pot manner and the yields range from moderate to excellent. A key nitropyrazolidine intermediate is characterized and a plausible mechanism is proposed.
IT 908329-93-1P 908329-95-3P 908329-96-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(one-pot regioselective synthesis of substituted pyrazoles from N-monosubstituted hydrazones and nitroolefins)
RN 908329-93-1 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-1-methyl-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

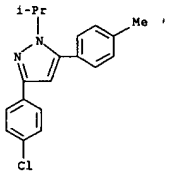


RN 908329-95-3 CAPLUS
CN 1H-Pyrazole, 3-(4-chlorophenyl)-5-(4-methylphenyl)-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

L26 ANSWER 2 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

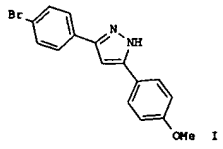


RN 908329-96-4 CAPLUS
CN 1H-Pyrazole, 3-(4-chlorophenyl)-1-(1-methylethyl)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



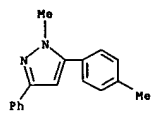
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 3 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:504334 CAPLUS
DOCUMENT NUMBER: 145:8083
TITLE: 1,3-Diketones from Acid Chlorides and Ketones: A Rapid and General One-Pot Synthesis of Pyrazoles
AUTHOR(S): Heller, Stephen T.; Natarajan, Swaminathan R.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Organic Letters (2006), 8(13), 2675-2678
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



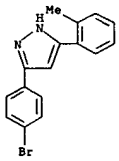
I

AB 1,3-Diketones were synthesized directly from ketones and acid chlorides and were then converted in situ into pyrazoles, e.g. I, by the addition of hydrazine. This method is extremely fast, general, and chemoselective, allowing for the synthesis of previously inaccessible pyrazoles and synthetically demanding pyrazole-containing fused rings.
IT 66870-43-7P 888482-91-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazoles via 1,3-diketones from acid chlorides and ketones)
RN 66870-43-7 CAPLUS
CN 1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 888482-91-5 CAPLUS
CN 1H-Pyrazole, 3-(4-bromophenyl)-5-(2-methylphenyl)- (9CI) (CA INDEX NAME)

L26 ANSWER 3 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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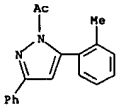
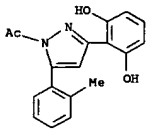
L26 ANSWER 4 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:473090 CAPLUS
DOCUMENT NUMBER: 145:95779
TITLE: Synthesis and molecular modelling of novel substituted-4,5-dihydro-(1H)-pyrazole derivatives as potent and highly selective monoamine oxidase-A inhibitors
AUTHOR(S): Chimenti, Franco; Bolasco, Adriana; Manna, Fedele; Secci, Daniela; Chimenti, Paola; Granese, Arianna; Befani, Olivia; Turini, Paola; Alcaro, Stefano; Ortuso, Francesco
CORPORATE SOURCE: Dipartimento di Studi di Chimica e Tecnologia delle Sostanze Biologicamente Attive, Universita degli Studi di Roma "La Sapienza", Rome, 00185, Italy
SOURCE: Chemical Biology & Drug Design (2006), 67(3), 206-214
CODEN: CBDDAL; ISSN: 1747-0277
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:95779
AB This report describes novel pyrazoline derivs. investigated for their ability to selectively inhibit the activity of the A and B isoforms of monoamine oxidase. These new synthetic compds. proved to be reversible, potent, and selective inhibitors of monoamine oxidase-A rather than of monoamine oxidase-B, and are promising candidates to further advance drug discovery efforts. The most active compds. show inhibitory activity on monoamine oxidase-A in the 1.0 + 10-8-8.6 + 10-9 M range. Moreover, it should be pointed out that for some compds. a high IC50 ≥ 10-9 M value is associated with a high A-selectivity (Selectivity Index monoamine oxidase-B/monoamine oxidase-A in the 10 000-12 500 range). Further insight to understand enzyme-inhibitor mol. interaction was obtained by docking expts. with the monoamine oxidase-A and monoamine oxidase-B isoforms.
IT 895138-49-5P 895138-50-8P 895138-51-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Synthesis and mol. modeling of novel substituted-4,5-dihydro-(1H)-pyrazole derivs. as potent and highly selective monoamine oxidase-A inhibitors)
RN 895138-49-5 CAPLUS
CN 1H-Pyrazole, 1-acetyl-5-(2-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

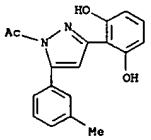


RN 895138-50-8 CAPLUS
CN 1H-Pyrazole, 1-acetyl-3-(2,6-dihydroxyphenyl)-5-(2-methylphenyl)- (9CI)

L26 ANSWER 4 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(CA INDEX NAME)

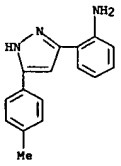


RN 895138-51-9 CAPLUS
CN 1H-Pyrazole, 1-acetyl-3-(2,6-dihydroxyphenyl)-5-(3-methylphenyl)- (9CI)
(CA INDEX NAME)

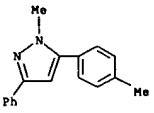


REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 5 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:358419 CAPLUS
Correction of: 2005:481374
DOCUMENT NUMBER: 145:123923
Correction of: 142:481542
TITLE: Acyclic and cyclic ureas
AUTHOR(S): Sartori, G.; Maggi, R.
CORPORATE SOURCE: Dipartimento di Chimica Organica, Industriale dell' Universita, Parma, I-43100, Italy
SOURCE: Science of Synthesis (2005), 18, 665-758
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review of the preparation of cyclic and acyclic ureas.
IT 178625-21-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cyclic and acyclic ureas)
RN 178625-21-3 CAPLUS
CN Benzenamine, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



L26 ANSWER 6 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:952848 CAPLUS
DOCUMENT NUMBER: 143:405840
TITLE: One-Pot Construction of Pyrazoles and Isoxazoles with Palladium-Catalyzed Four-Component Coupling
AUTHOR(S): Ahmed, Mohamed S. Mohamed; Kobayashi, Kei; Mori, Atsunori
CORPORATE SOURCE: Chemical Resources Laboratory, Tokyo Institute of Technology, Yokohama, 226-8503, Japan
SOURCE: Organic Letters (2005), 7(20), 4487-4489
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:405840
AB Four-component coupling of a terminal alkyne, hydrazine (hydroxylamine), carbon monoxide, and an aryl iodide furnishes pyrazole or isoxazole derivs. in the presence of a palladium catalyst. The reaction proceeds at room temperature and an ambient pressure of carbon monoxide in an aqueous solvent system.
IT 66870-43-7P, 1-Methyl-5-(4-methylphenyl)-3-phenyl-1H-pyrazole
RL: SPN (Synthetic preparation); PREP (Preparation)
(one-pot construction of pyrazoles and isoxazoles by palladium-catalyzed four-component coupling)
RN 66870-43-7 CAPLUS
CN 1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Karen Cheng

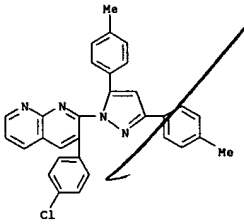
10526940species

L26 ANSWER 7 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:912268 CAPLUS
DOCUMENT NUMBER: 142:316748
TITLE: Hypervalent iodine mediated mild and efficient oxidation of pyrazolines to pyrazoles in solid state
AUTHOR(S): Mogilaiah, K.; Reddy, G. R.
CORPORATE SOURCE: Department of Chemistry, Kakatiya University, Warangal, 506 009, India
SOURCE: Oxidation Communications (2004), 27(3), 668-673
CODEN: OXCODW; ISSN: 0209-4541
PUBLISHER: SciBulCom Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:316748

AB An efficient and mild method for the oxidation of pyrazolinyl-1,8-naphthyridines to pyrazolyl-1,8-naphthyridines using iodobenzene diacetate in the solid state has been described. The yields are good and purity is high. The method is preparatively convenient and useful.

IT 848356-06-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(hypervalent iodine mediated mild and efficient oxidation of pyrazolines to pyrazoles in solid state)

RN 848356-06-9 CAPLUS
CN 1,8-Naphthyridine, 2-[3,5-bis(4-methylphenyl)-1H-pyrazol-1-yl]-3-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



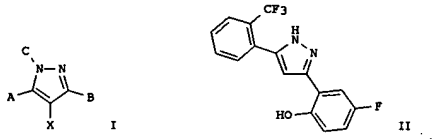
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:780671 CAPLUS
DOCUMENT NUMBER: 141:296010
TITLE: Preparation of substituted pyrazoles as modulators of ATP-binding cassette transporters
INVENTOR(S): Vangoor, Frederick F.; Hadida Ruah, Sarah S.; Singh, Ashvani K.; Olson, Eric R.; Makings, Lewis R.; Gonzalez, Jesus E., III; Rader, James A.; Chambers, Fred, III; Miller, Mark T.; Grootenhuis, Peter; Liu, Yahua
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 174 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004080972	A1	20040923	WO 2004-US7492	20040312
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005113423	A1	20050526	US 2004-800022	20040312
EP 1601657	A1	20051207	EP 2004-720345	20040312
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				

PRIORITY APPLN. INFO.: US 2003-453978P P 20030312
WO 2004-US7492 W 20040312

OTHER SOURCE(S): MARPAT 141:296010
GI

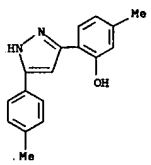


AB Pyrazoles I [A, B = (un)substituted aryl, heterocyclyl, cycloalkyl; C = H, (un)substituted aryl, heterocyclyl, cycloalkyl, alkyl, alkylcarbonyl, arylcarbonyl, heteroarylcarbonyl, heterocyclylcarbonyl, or aminocarbonyl; X = H, (un)substituted alkyl, aryl, heterocyclyl, heteroaryl, or ω-substituted n-alkyl] such as II are prepd. as inhibitors of ATP-binding cassette (ABC) transporters such as the cystic fibrosis transmembrane conductance regulator (CFTR) for use in the treatment of conditions such as cystic fibrosis, immunodeficiency, inflammatory disease, chronic obstructive pulmonary disease, chronic pancreatitis, or pneumonia. 4-Trifluoromethylbenzoyl chloride and 2-hydroxy-5-fluoroacetophenone are stirred in pyridine for 12 h, after which potassium hydroxide is added and the mixt. stirred for 12 h; addn. of hydrazine hydrate to a soln. of the product obtained in the first step in ethanol and heating at reflux for 3 h yields II in 30% overall yield as a yellow cryst. solid. II modulates ΔF508-CFTR at ≥75% of the effect of genistein on the same receptor. Data on the relative modulation of ΔF508-CFTR by some compds. of the invention as compared to genistein is provided.

L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

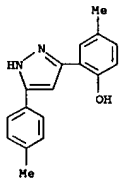
IT 416877-12-8P 416880-94-9P 423735-70-0P 423746-90-1P 423750-83-8P 423752-83-4P 423753-85-9P 763132-75-8P 763132-82-7P 763132-90-7P 763132-99-6P 763133-01-3P 763133-12-6P 763133-25-1P 763133-27-3P 763133-63-7P 763133-84-2P 763133-85-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrazoles as modulators of ATP-binding cassette transporters such as the cystic fibrosis transmembrane conductance regulator for treatment of diseases such as cystic fibrosis, immunodeficiency, and pneumonia)

RN 416877-12-8 CAPLUS
CN Phenol, 5-methyl-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

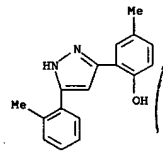


RN 416880-94-9 CAPLUS
CN Phenol, 4-methyl-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

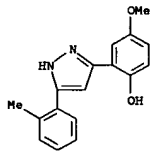
L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 423735-70-0 CAPLUS
CN Phenol, 4-methyl-2-[5-(2-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 423746-90-1 CAPLUS
CN Phenol, 4-methoxy-2-[5-(2-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

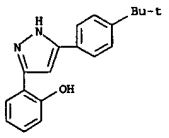


RN 423750-83-8 CAPLUS
CN Phenol, 2-[5-[4-(1,1-dimethylethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

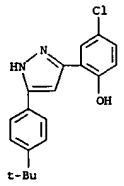
Karen Cheng

10526940species

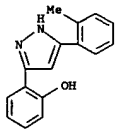
L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 423752-83-4 CAPLUS
CN Phenol, 4-chloro-2-[5-[4-(1,1-dimethylethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

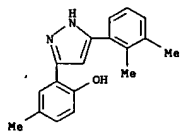


RN 423753-85-9 CAPLUS
CN Phenol, 2-[5-(2-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

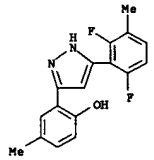


RN 763132-75-8 CAPLUS
CN Phenol, 4-methyl-2-[5-[3-methyl-4-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

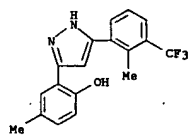
L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 763133-01-3 CAPLUS
CN Phenol, 2-[5-(2,6-difluoro-3-methylphenyl)-1H-pyrazol-3-yl]-4-methyl- (9CI) (CA INDEX NAME)

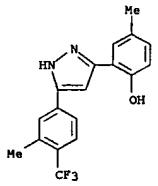


RN 763133-12-6 CAPLUS
CN Phenol, 4-methyl-2-[5-[2-methyl-3-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

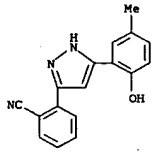


RN 763133-25-1 CAPLUS
CN Benzenesulfonamide, N,N-diethyl-4-[5-(2-hydroxy-5-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

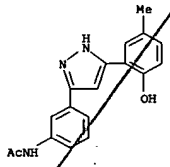
L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 763132-82-7 CAPLUS
CN Benzonitrile, 2-[5-(2-hydroxy-5-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

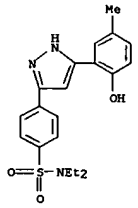


RN 763132-90-7 CAPLUS
CN Acetamide, N-[3-[5-(2-hydroxy-5-methylphenyl)-1H-pyrazol-3-yl]phenyl]- (9CI) (CA INDEX NAME)

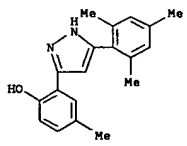


RN 763132-99-6 CAPLUS
CN Phenol, 2-[5-(2,3-dimethylphenyl)-1H-pyrazol-3-yl]-4-methyl- (9CI) (CA INDEX NAME)

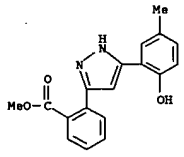
L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 763133-27-3 CAPLUS
CN Phenol, 4-methyl-2-[5-(2,4,6-trimethylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



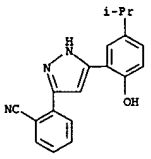
RN 763133-63-7 CAPLUS
CN Benzoic acid, 2-[5-(2-hydroxy-5-methylphenyl)-1H-pyrazol-3-yl]-, methyl ester (9CI) (CA INDEX NAME)

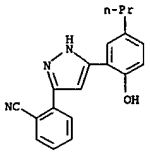


RN 763133-84-2 CAPLUS
CN Benzonitrile, 2-[5-[2-hydroxy-5-(1-methylethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

Karen Cheng

L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

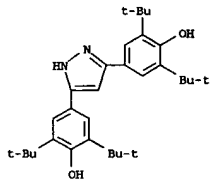




RN 763133-85-3 CAPLUS
CN Benzonitrile, 2-[5-(2-hydroxy-5-propylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

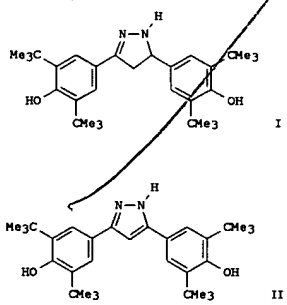
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 9 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(Biological study); PREP (Preparation)
(prepn. and low-d. lipoprotein peroxidn. inhibition of bis[di(t-butyl)hydroxyphenyl]pyrazole via oxidn. of bis[di(t-butyl)hydroxyphenyl]pyrazoline)
RN 721447-01-4 CAPLUS
CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis[2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



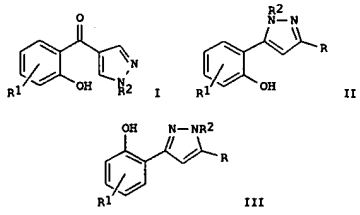
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 9 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:362548 CAPLUS
DOCUMENT NUMBER: 141:106411
TITLE: Novel 3,5-diarylpyrazolines and pyrazole as low-density lipoprotein (LDL) oxidation inhibitor
AUTHOR(S): Jeong, Tae-Sook; Kim, Kyung Soon; Kim, Ju-Ryoung; Cho, Kyung-Hyun; Lee, Sangku; Lee, Woo Song
CORPORATE SOURCE: National Research Laboratory of Lipid Metabolism & Atherosclerosis, Korea Research Institute of Bioscience and Biotechnology, Daejeon, 305-333, S. Korea
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(11), 2719-2723
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:106411
GI



AB 2,3-Diarylpyrazolines, e.g., I, and -pyrazole II were synthesized by cyclocondensation of chalcones with hydrazine, and tested for their LDL-oxidation inhibition activity. The tested compds. showed significant LDL-antioxidant activities in the TBARS assay, the lag time of conjugated diene production, the relative electrophoretic mobility (REM) of ox-LDL, the apoB-100 fragmentation, and the macrophage-mediated LDL oxidation I and II were found to be the most active compds. as an inhibitor of LDL oxidation, and I (IC50 = 0.1 μM) was 6-fold more potent than probucol (IC50 = 0.6 μM) in the TBARS assay.
IT 721447-01-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL

L26 ANSWER 10 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:347011 CAPLUS
DOCUMENT NUMBER: 141:332110
TITLE: Design and synthesis of two pyrazole libraries based on o-hydroxyacetophenones
AUTHOR(S): Borrell, Jose I.; Schuler, Elisabeth; Teixido, Jordi; Michelotti, Enrique L.
CORPORATE SOURCE: Institut Quimic de Sarria, Grup d'Enginyeria Molecular, Universitat Ramon Llull, Barcelona, E-08017, Spain
SOURCE: Molecular Diversity (2004), 8(2), 147-157
CODEN: MODIF4; ISSN: 1381-1991
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:332110
GI

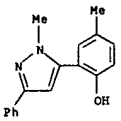


AB Two new solid-phase syntheses of substituted pyrazoles are described. The first includes supporting an o-hydroxyacetophenone on Merrifield resin, Vilsmeier-Haack formylation on the Me group and cyclization with a substituted hydrazine to afford a pyrazole ring with two diversity centers, e.g. I [R1 = H, 4-F, 3,4-(MeO)2, etc., R2 = Ph, n-Pr, 2-benzothiazolyl, etc.]. The second starts from o-hydroxyacetophenone supported on Wang resin, which undergoes a Claisen condensation with a carboxylic acid ester to yield a 1,3-dicarbonyl compound that cyclizes to a pyrazole using a hydrazine, II and III (R = H, Me, Ph). Both methods have been used to synthesize two small pyrazole libraries.
IT 771483-85-3P 771484-12-9P
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)
(design and solid-phase syntheses of pyrazole libraries using o-hydroxyacetophenones, their fungicidal, insecticidal, and herbicidal activities)
RN 771483-85-3 CAPLUS
CN Phenol, 4-methyl-2-(1-methyl-3-phenyl-1H-pyrazol-5-yl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 771483-84-2

L26 ANSWER 10 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C17 H16 N2 O



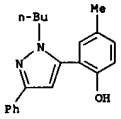
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 771484-12-9 CAPLUS
CN Phenol, 2-(1-butyl-3-phenyl-1H-pyrazol-5-yl)-4-methyl-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 771484-11-8
CMF C20 H22 N2 O



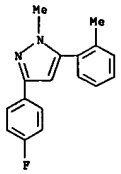
CM 2

CRN 76-05-1
CMF C2 H F3 O2

L26 ANSWER 10 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

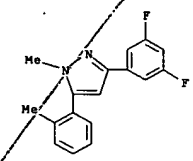
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 11 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:302811 CAPLUS
DOCUMENT NUMBER: 141:23470
TITLE: Regioselective rapid analog syntheses of 1-methyl-3,5-diarylpyrazoles via palladium-catalyzed coupling to 3(5)-pyrazolyl nonaflates
AUTHOR(S): Bourrain, Sylvie; Ridgill, Mark; Collins, Ian
CORPORATE SOURCE: Department of Medicinal Chemistry, The Neuroscience Research Centre, Merck Sharp and Dohme Research Laboratories, Essex, CM20 2QR, UK
SOURCE: Synlett (2004), (5), 795-798
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:23470
AB Regioselective rapid analog syntheses of 1-methyl-3,5-diarylpyrazoles were developed, based on Pd-catalyzed couplings to 1-methyl-3(5)-arylpyrazole nonaflates, which offered an advantage in hydrolytic stability over the corresponding triflates. The new bifunctional reagent 1-methyl-3-bromo-pyrazol-5-yl nonaflate underwent highly chemoselective Pd-catalyzed couplings to the nonaflate, followed by Suzuki couplings to the bromide, allowing sequential, regioselective introduction of the two aryl substituents.
IT 699010-12-3P 699010-21-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective synthesis of 1-methyl-3,5-diarylpyrazoles through palladium-catalyzed coupling of 1-methyl-3-bromo-pyrazol-5-yl nonaflates)
RN 699010-12-3 CAPLUS
CN 1H-Pyrazole, 3-(4-fluorophenyl)-1-methyl-5-(2-methylphenyl)- (9CI) (CA INDEX NAME)



RN 699010-21-4 CAPLUS
CN 1H-Pyrazole, 3-(3,5-difluorophenyl)-1-methyl-5-(2-methylphenyl)- (9CI) (CA INDEX NAME)

L26 ANSWER 11 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10526940species

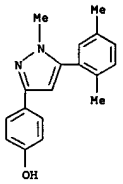
L26 ANSWER 12 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:211991 CAPLUS
DOCUMENT NUMBER: 140:264528
TITLE: NR3B1 nuclear receptor-binding 3-substituted pyrazole derivatives, and therapeutic uses
INVENTOR(S): Deuschle, Ulrich; Heck, Stefanie; Kober, Ingo; Bauer, Ulrike; Balogh, Imoia
PATENT ASSIGNEE(S): Lion Bioscience A.-G., Germany
SOURCE: Eur. Pat. Appl., 45 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1398029	A1	20040317	EP 2002-20256	20020910
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
WO 2004024148	A1	20040325	WO 2003-EP7066	20030702
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003250877	A1	20040430	AU 2003-250877	20030702
US 2006148876	A1	20060706	US 2005-526940	20051021
PRIORITY APPLN. INFO.:			EP 2002-20256 A	20020910
			WO 2003-EP7066 W	20030702

OTHER SOURCE(S): MARPAT 140:264528
AB The invention discloses pyrazole derivs. which bind to the NR3B1 receptor and act as antagonists of the NR3B1 receptor. The invention further relates to the treatment of diseases and/or conditions through binding of the nuclear receptor by the compds., as well as the production of medicaments using the compds.
IT 362006-35-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(NR3B1 nuclear receptor-binding pyrazole derivs., and therapeutic uses)
RN 362006-35-7 CAPLUS
CN Phenol, 4-[5-(2,5-dimethylphenyl)-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

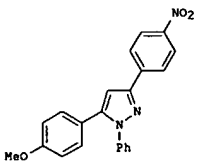
current app.

L26 ANSWER 12 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



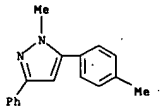
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 13 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:58889 CAPLUS
DOCUMENT NUMBER: 140:253486
TITLE: Regioselective synthesis of 1,3,5-substituted pyrazoles from acetylenic ketones and hydrazines
AUTHOR(S): Bishop, Brian C.; Brands, Karel M. J.; Gibb, Andrew D.; Kennedy, Derek J.
CORPORATE SOURCE: Merck Sharp & Dohme Research Laboratories, Department of Process Research, Hertfordshire, EN11 9BU, UK
SOURCE: Synthesis (2004), (1), 43-52
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:253486
GI



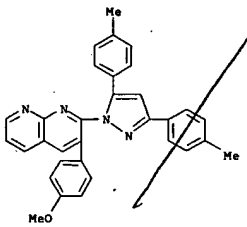
I

AB The synthesis of 1,3,5-trisubstituted pyrazoles, e.g., I, from the reaction of acetylenic ketones with substituted hydrazines, is reported. The reactions were shown to be highly regioselective regardless of the nature of the substituents in the substrates and afforded essentially single pyrazole isomers in excellent yields.
IT 66870-43-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective preparation of pyrazoles via heterocyclization of diarylpropynones with hydrazines followed by dehydration)
RN 66870-43-7 CAPLUS
CN 1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 14 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:854945 CAPLUS
DOCUMENT NUMBER: 140:199252
TITLE: Mild and efficient oxidation of pyrazolinyl-1,8-naphthyridines to pyrazolyl-1,8-naphthyridines mediated by cerium(IV) ammonium nitrate under microwave irradiation
AUTHOR(S): Mogilaiah, K.; Reddy, N. Vasudeva; Rao, R. Babu
CORPORATE SOURCE: Department of Chemistry, Kakatiya University, Warangal, 506 009, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2003), 42B(10), 2618-2621
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:199252
AB Cerium(IV) ammonium nitrate (CAN) was used as an effective oxidizing agent for the oxidation of pyrazolinyl-1,8-naphthyridines to the corresponding pyrazolyl-1,8-naphthyridines under microwave irradiation with high yields.
IT 663155-83-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(oxidation of pyrazolinyl-1,8-naphthyridines to pyrazolyl-1,8-naphthyridines using cerium(IV) ammoniumnitrate oxidant under microwave irradiation)
RN 663155-83-7 CAPLUS
CN 1,8-Naphthyridine, 2-[3,5-bis(4-methylphenyl)-1H-pyrazol-1-yl]-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



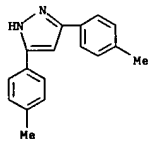
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Karen Cheng

10526940species

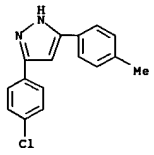
Check Dates

L26 ANSWER 15 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:855864 CAPLUS
DOCUMENT NUMBER: 139:214344
TITLE: Product class 1: pyrazoles
AUTHOR(S): Stanovnik, B.; Svete, J.
CORPORATE SOURCE: Faculty of Chemistry and Chemical Technology, Division of Organic Chemistry, Ljubljana, 61000, Slovenia
SOURCE: Science of Synthesis (2002), 12, 15-225
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. Methods for preparing pyrazoles are reviewed including cyclization, ring transformation, aromatization and substituent modifications.
IT 93330-77-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazoles via cyclization, ring transformation, aromatization and substituent modifications)
RN 93330-77-9 CAPLUS
CN 1H-Pyrazole, 3,5-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)



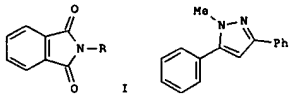
REFERENCE COUNT: 909 THERE ARE 909 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 16 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:150071 CAPLUS
DOCUMENT NUMBER: 137:33270
TITLE: Novel tandem reactions of 2,2'-sulfonylbis(1,3-diarylprop-2-en-1-ones) with hydrazine. Formation of 3,6-diarylpyridazines and 3,5-diarylpyrazoles
AUTHOR(S): Gnanadeepam, M.; Selvaraj, S.; Perumal, S.; Renuga, S.
CORPORATE SOURCE: Department of Chemistry, Fatima College, Madurai, 625 018, India
SOURCE: Tetrahedron (2002), 58(11), 2227-2230
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:33270
AB The 2,2'-sulfonylbis(1,3-diarylprop-2-en-1-ones) undergo tandem reactions with hydrazine affording 3,6-diarylpyridazines and 3,5-diarylpyrazoles unexpectedly, the latter predominating.
IT 131138-54-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 3,6-diarylpyridazines and 3,5-diarylpyrazoles by tandem reactions of sulfonylbis(diarylpropenones) with hydrazine)
RN 131138-54-0 CAPLUS
CN 1H-Pyrazole, 3-(4-chlorophenyl)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

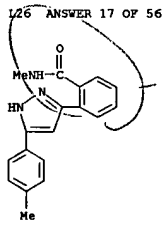
L26 ANSWER 17 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:71213 CAPLUS
DOCUMENT NUMBER: 136:401679
TITLE: Regioselective synthesis of pyrazoles via the ring cleavage of 3-substituted N-alkylated 3-hydroxyisoindolin-1-ones
AUTHOR(S): Chang, Kyu-Tae; Choi, Yong Hyun; Kim, Seung-Ho; Yoon, Yong-Jin; Lee, Woo Song
CORPORATE SOURCE: Proteome Research Laboratory, Korea Research Institute of Bioscience and Biotechnology, Taejon, 305-333, S. Korea
SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2002), (2), 207-210
CODEN: JCSPCE; ISSN: 1472-7781
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:401679
GI



I II

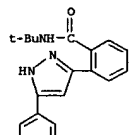
AB N-Alkyl (Me, Et, iPr, tBu)-substituted phthalimides I (R = Me, Et, i-Pr, t-Bu) were easily transformed to mono-, di-, or tri-substituted pyrazoles, e.g., II via a one-pot addition-decyclization-cyclocondensation process. The regiochem. of the pyrazole ring was determined by X-ray crystallog. anal. and 1H NOE expts.
IT 431877-70-2P 431877-76-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazoles from N-alkylphthalimides via addition of lithium alkylacetylides, ring cleavage of intermediate N-alkylhydroxyisoindolinones and subsequent regioselective cyclocondensation with hydrazines)
RN 431877-70-2 CAPLUS
CN Benzamide, N-methyl-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L26 ANSWER 17 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



subst. phenyl.

RN 431877-76-8 CAPLUS
CN Benzamide, N-(1,1-dimethylethyl)-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

102b - claims 1 & 2

103 - claim 3.

Karen Cheng

10526940species

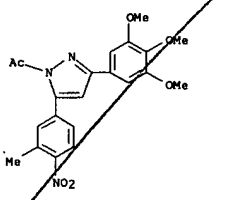
L26 ANSWER 18 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:749722 CAPLUS
DOCUMENT NUMBER: 136:47977
TITLE: New antimitotic agents with activity in multidrug-resistant cell lines and in vivo efficacy in murine tumor models
AUTHOR(S): Szczepankiewicz, Bruce G.; Liu, Gang; Jae, Hwan-Soo; Tasker, Andrew S.; Gunawardana, Indrani W.; von Geldern, Thomas W.; Gwaltney, Stephen L., II; Wu-Wong, J. Ruth; Gehrke, Laura; Chiou, William J.; Credo, R. Bruce; Alder, Jeffery D.; Nukkala, Michael A.; Zielinski, Nicolette A.; Jarvis, Ken; Mollison, Karl W.; Frost, David J.; Bauch, Joy L.; Hui, Yu Hua; Claiborne, Akiyo K.; Li, Qun; Rosenberg, Saul H.
CORPORATE SOURCE: Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(25), 4416-4430
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:47977

AB During a screen for compds. that could inhibit cell proliferation, a series of new tubulin-binding compds. was identified with the discovery of oxadiazoline A-105972. This compound showed good cytotoxic activity against non-multi-drug-resistant and multi-drug-resistant cancer cell lines, but its utility in vivo was limited by a short half-life. Medicinal chemical efforts led to the discovery of indolyloxazoline A-259745, which maintained all of the in vitro activity seen with oxadiazoline 1, but also demonstrated a better pharmacokinetic profile, and dose-dependent in vivo activity. Over a 28 day study, indolyloxazoline A-259745 increased the life span of tumor-implanted mice by up to a factor of 3 upon oral dosing. This compound, and others of its structural class, may prove to be useful in the development of new chemotherapeutic agents to treat human cancers.

IT 380922-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(antimitotic agents with activity in multidrug-resistant cell lines and in vivo efficacy in murine tumor models)

RN 380922-11-2 CAPLUS
CN 1H-Pyrazole, 1-acetyl-5-(3-methyl-4-nitrophenyl)-3-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

L26 ANSWER 18 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



R1

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

claim 1,

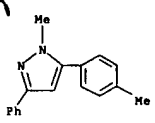
L26 ANSWER 19 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:658144 CAPLUS
DOCUMENT NUMBER: 135:344418
TITLE: Regioselective Synthesis of Polysubstituted Pyrazoles and Isoxazoles
AUTHOR(S): Katritzky, Alan R.; Wang, Mingyi; Zhang, Suoming; Voronkov, Michael V.; Steel, Peter J.
CORPORATE SOURCE: Department of Chemistry Center for Heterocyclic Compounds, University of Florida, Gainesville, FL, 32611-7200, USA
SOURCE: Journal of Organic Chemistry (2001), 66(20), 6787-6791
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:344418

AB A regioselective synthesis has been developed for the preparation of unsym. 1,3,5-triaryl-4-alkylpyrazolines and -pyrazoles by treatment of α-benzotriazolyl-α,β-unsatd. ketones with monosubstituted hydrazines followed by alkylation at the 4-position of the pyrazoline ring. Reaction of α-benzotriazolyl-α,β-unsatd. ketones with hydroxylamine gives 3,5-disubstituted isoxazoles regioselectively.

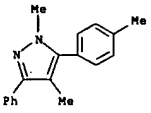
IT 66870-43-7P 371772-74-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective synthesis of polysubstituted pyrazoles and isoxazoles)

RN 66870-43-7 CAPLUS
CN 1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

not subst. phenyl



RN 371772-74-6 CAPLUS
CN 1H-Pyrazole, 1,4-dimethyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

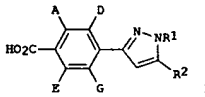


REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 20 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:553563 CAPLUS
DOCUMENT NUMBER: 133:164050
TITLE: Preparation of diarylpyrazolecarboxylates as erythropoietin sensitizers.
INVENTOR(S): Stoltefuss, Jurgen; Braunlich, Gabriele; Hinzen, Berthold; Kramer, Thomas; Fernerstorfer, Josef; Studemann, Thomas; Nielsch, Ulrich; Bechem, Martin; Lohrmann, Emanuel; Gerdes, Christoph; Sperzel, Michael; Lustig, Klemens; Mayr, Lorenz
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000046208	A1	20000810	WO 2000-EP511	20000124
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19904406	A1	20000810	DE 1999-19904406	19990204
CA 2361816	A1	20000810	CA 2000-2361816	20000124
EP 1150958	A1	20011107	EP 2000-910605	20000124
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002536365	T	20021029	JP 2000-597278	20000124
PRIORITY APPLN. INFO.:			DE 1999-19904406 A	19990204
			WO 2000-EP511 W	20000124

OTHER SOURCE(S): MARPAT 133:164050
GI



I

AB Title compds. [I; A, D, E, G = H, halo, CF3, OH, alkyl, alkoxy; R1 = H, alkyl; R2 = (substituted) naphthyl, (benzo-fused) heterocyclyl], were prepared Thus, 1-(4-methoxycarbonylphenyl)-3-(4-trifluoromethylphenyl)-1,3-propanedione was refluxed with N2H4 to give 3-(4-methoxycarbonylphenyl)-5-(4-trifluoromethylphenyl)pyrazole. This was treated with NaH/MeI in THF to give 3-(4-methoxycarbonylphenyl)-1-methyl-5-(4-

Karen Cheng

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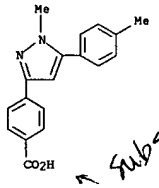
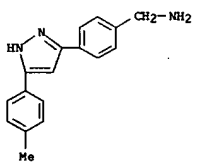
L26 ANSWER 20 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
trifluoromethylphenyl)pyrazole. This was refluxed with aq. NaOH in EtOH to give 3-(4-carboxyphenyl)-1-methyl-5-(4-trifluoromethylphenyl)pyrazole. The latter at 10 μM gave an 86% increase in erythrocyte precursor cells.
IT 287951-36-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diarylpyrazolecarboxylates as erythropoietin sensitizers)
RN 287951-36-4 CAPLUS
CN Benzoic acid, 4-[1-methyl-5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



Subst. phenyl. claim 1 & 3.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 21 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrazolylbenzylamines for treatment of anemia)
RN 287727-26-8 CAPLUS
CN Benzenemethanamine, 4-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



claim 1-2 - 103 claim 3.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 21 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:553561 CAPLUS
DOCUMENT NUMBER: 133:150559
TITLE: Preparation of pyrazolylbenzylamines for treatment of anemia.
INVENTOR(S): Stoltefuss, Jurgen; Braunlich, Gabriele; Hinzen, Berthold; Kramer, Thomas; Pernerstorfer, Josef; Studemann, Thomas; Nielsch, Ulrich; Bechem, Martin; Lohrmann, Emanuel; Gerdes, Christoph; Sperzel, Michael; Lustig, Klemens; Mayr, Lorenz
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000046206	A1	20000810	WO 2000-EP503	20000124
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19904396	A1	20000810	DE 1999-19904396	19990204
PRIORITY APPLN. INFO.:			DE 1999-19904396 A	19990204
OTHER SOURCE(S):	MARPAT 133:150559			

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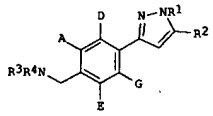


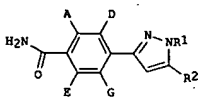
I

AB Title compds. [I; A, D, E, G = H, halo, CF3, OH, alkyl, alkoxy; R1 = H, alkyl; R2 = (substituted) aryl, 5-6 membered (benzo-condensed) heteroaryl; R3, R4 = H, acyl, alkyl, aminocarbonyl], were prepared as erythropoietin sensitizers (no data). Thus, 3-(4-aminocarbonylphenyl)-5-(4-methoxyphenyl)-1-methylpyrazole was stirred with BH3 in THF to give 3-(4-aminomethylphenyl)-5-(4-methoxyphenyl)-1-methylpyrazole.
IT 287727-26-8P

L26 ANSWER 22 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:553481 CAPLUS
DOCUMENT NUMBER: 133:150558
TITLE: Preparation of pyrazolylarylcarboxamides for treatment of anemia.
INVENTOR(S): Stoltefuss, Jurgen; Braunlich, Gabriele; Hinzen, Berthold; Kramer, Thomas; Pernerstorfer, Josef; Studemann, Thomas; Nielsch, Ulrich; Bechem, Martin; Lohrmann, Emanuel; Gerdes, Christoph; Sperzel, Michael; Lustig, Klemens; Mayr, Lorenz
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000045894	A2	20000810	WO 2000-EP519	20000124
WO 2000045894	A3	20010419		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19904397	A1	20000810	DE 1999-19904397	19990204
CA 2361636	A1	20000810	CA 2000-2361636	20000124
EP 1148879	A2	20011031	EP 2000-909096	20000124
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002536348	T	20021029	JP 2000-597013	20000124
PRIORITY APPLN. INFO.:			DE 1999-19904397 A	19990204
			WO 2000-EP519 W	20000124
OTHER SOURCE(S):	MARPAT 133:150558			

GI



I

AB Use of title compds. [I; A, D, E, G = H, halo, CF3, OH, alkyl, alkoxy; R1 = H, alkyl; R2 = (substituted) aryl, 5-6 membered (benzo-condensed) heterocyclyl] as drugs for treatment of disease, particularly anemia, is claimed (no data). Acetophenone-4-carboxylic acid supported on Tentagel SAM resin was heated at 90° with Me 4-bromobenzoate and NaH in

Karen Cheng

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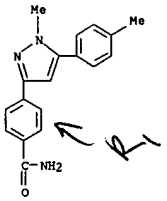
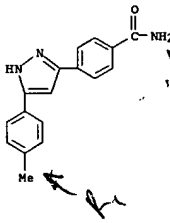
L26 ANSWER 22 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
dimethylacetamide; the product was stirred with MeNHNH2 in dimethylacetamide at 70° followed by resin cleavage with CF3CO2H in CH2Cl2 to give 3-(aminocarbonylphenyl)-5-(4-bromophenyl)-1-methylpyrazole.
IT 287395-67-9P 287395-72-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolylarylcarboxamides for treatment of anemia)
RN 287395-67-9 CAPLUS
CN Benzamide, 4-[1-methyl-5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



Claims 1-3

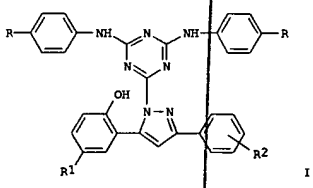
RN 287395-72-6 CAPLUS
CN Benzamide, 4-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



not alkylphenyl for R3

1026 - claims 1-2
103 - claim 3.

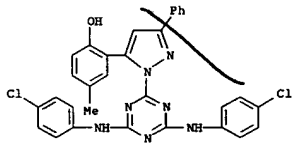
L26 ANSWER 23 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:545310 CAPLUS
DOCUMENT NUMBER: 134:131499
TITLE: Synthesis and biological activity of 2,4-bis(substituted anilino)-6-(pyrazolyl)-s-triazines
AUTHOR(S): Mane, D. V.; Chavan, V. P.; Mane, A. S.; Bhawsar, S. B.; Shingare, M. S.
CORPORATE SOURCE: P.G. Dept. of Chemistry S.C.S. College, Dr. B.A. Marathawada University, Aurangabad, 431 004, India
SOURCE: Indian Journal of Heterocyclic Chemistry (2000), 9(4), 271-274
CODEN: IJCHEI; ISSN: 0971-1627
PUBLISHER: Prof. R. S. Varma
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:131499
GI



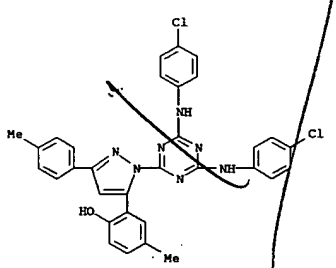
I

AB Title compds. such as I (R = Cl, NO2, Me, EtO; R1 = Me, Cl; R2 = H, 4-Me, 4-OMe, 3-Cl, 4-NO2) were prepared These compds. possessed promising antibacterial and antifungal activities.
IT 321896-92-8P 321896-93-9P 321896-95-1P
321896-96-2P 321897-05-6P 321897-06-7P
321897-07-8P 321897-14-7P 321897-15-8P
321897-16-9P 321897-17-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(2,4-bis(substituted anilino)-6-(pyrazolyl)-s-triazines and their antimicrobial activity)
RN 321896-92-8 CAPLUS
CN Phenol, 2-[1-[4,6-bis[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-3-phenyl-1H-pyrazol-5-yl]-4-methyl- (9CI) (CA INDEX NAME)

L26 ANSWER 23 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

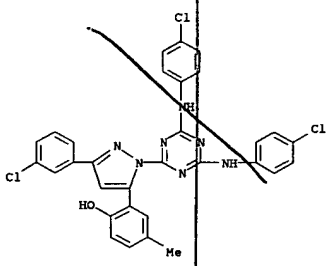


RN 321896-93-9 CAPLUS
CN Phenol, 2-[1-[4,6-bis[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-3-(4-methylphenyl)-1H-pyrazol-5-yl]-4-methyl- (9CI) (CA INDEX NAME)

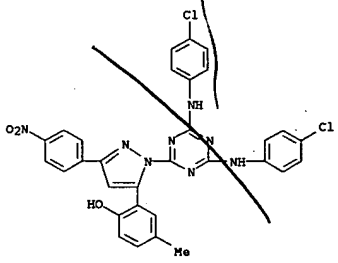


RN 321896-95-1 CAPLUS
CN Phenol, 2-[1-[4,6-bis[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-3-(3-chlorophenyl)-1H-pyrazol-5-yl]-4-methyl- (9CI) (CA INDEX NAME)

L26 ANSWER 23 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



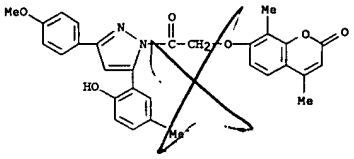
RN 321896-96-2 CAPLUS
CN Phenol, 2-[1-[4,6-bis[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-3-(4-nitrophenyl)-1H-pyrazol-5-yl]-4-methyl- (9CI) (CA INDEX NAME)



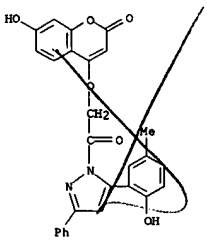
RN 321897-05-6 CAPLUS
CN Phenol, 2-[1-[4,6-bis[(4-nitrophenyl)amino]-1,3,5-triazin-2-yl]-3-(4-methoxyphenyl)-1H-pyrazol-5-yl]-4-methyl- (9CI) (CA INDEX NAME)

Karen Cheng

L26 ANSWER 24 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

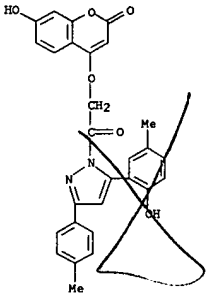


RN 263407-72-3 CAPLUS
CN 1H-Pyrazole, 5-(2-hydroxy-5-methylphenyl)-1-[[(7-hydroxy-2-oxo-2H-1-benzopyran-4-yl)oxy]acetyl]-3-phenyl- (9CI) (CA INDEX NAME)

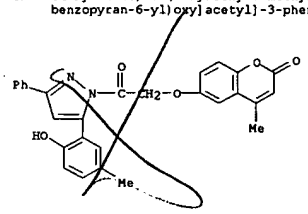


RN 263407-73-4 CAPLUS
CN 1H-Pyrazole, 5-(2-hydroxy-5-methylphenyl)-1-[[(7-hydroxy-2-oxo-2H-1-benzopyran-4-yl)oxy]acetyl]-3-(4-methylphenyl)- (9CI) (CA INDEX NAME)

L26 ANSWER 24 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

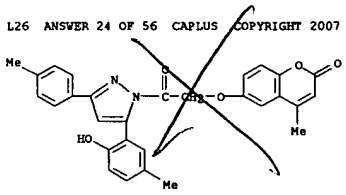


RN 263407-80-3 CAPLUS
CN 1H-Pyrazole, 5-(2-hydroxy-5-methylphenyl)-1-[[(4-methyl-2-oxo-2H-1-benzopyran-6-yl)oxy]acetyl]-3-phenyl- (9CI) (CA INDEX NAME)

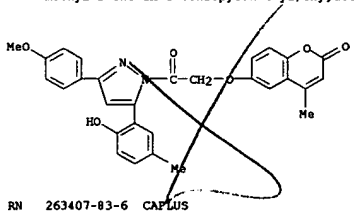


RN 263407-81-4 CAPLUS
CN 1H-Pyrazole, 5-(2-hydroxy-5-methylphenyl)-1-[[(4-methyl-2-oxo-2H-1-benzopyran-6-yl)oxy]acetyl]-3-(4-methylphenyl)- (9CI) (CA INDEX NAME)

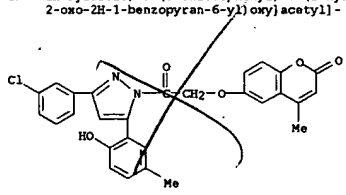
L26 ANSWER 24 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263407-82-5 CAPLUS
CN 1H-Pyrazole, 5-(2-hydroxy-5-methylphenyl)-3-(4-methoxyphenyl)-1-[[(4-methyl-2-oxo-2H-1-benzopyran-6-yl)oxy]acetyl]- (9CI) (CA INDEX NAME)



RN 263407-83-6 CAPLUS
CN 1H-Pyrazole, 3-(3-chlorophenyl)-5-(2-hydroxy-5-methylphenyl)-1-[[(4-methyl-2-oxo-2H-1-benzopyran-6-yl)oxy]acetyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

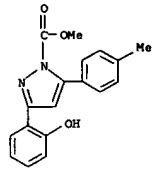
L26 ANSWER 25 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:526163 CAPLUS
DOCUMENT NUMBER: 131:286138
TITLE: A new series of proton/charge transfer molecules: synthesis and spectral studies of 2-(5-aryl-1-carbomethoxy-1H-pyrazol-3-yl)phenols
AUTHOR(S): Rampey, Mary E.; Halkyard, Carrie E.; Williams, Angela R.; Angel, April J.; Hurst, Douglas R.; Townsend, Jessica D.; Finefrock, Anne E.; Beam, Charles F.; Studer-Martinez, Shannon L.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, College of Charleston, Charleston, SC, 29424, USA
SOURCE: Photochemistry and Photobiology (1999), 70(2), 176-183
CODEN: PHCBAP; ISSN: 0031-8655
PUBLISHER: American Society for Photobiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The carbomethoxyhydrazone of 2'-hydroxyacetophenone was trilithiated with excess lithium diisopropylamide and C-acylated with a variety of benzoate esters followed by acid cyclization of the intermediates to 2-(5-aryl-1-carbomethoxy-1H-pyrazol-3-yl)phenols [3-(2-hydroxyphenyl)-1H-pyrazoles]. The products were characterized by Fourier transform-IR, 1H NMR, 13C NMR, UV-visible absorption and fluorescence. All the derivs. in n-heptane have an absorption maximum at .apprx.304 nm and an extremely weak (Φf = 10-4) fluorescence with maxima in the range of 335-460 nm. The broad range of fluorescence maxima and fluorescence quantum yields is attributed to varying contributions of charge transfer that are dependent on both the identity of the substituent and solvent polarity. A phenomenally large Stokes-shifted fluorescence maximum at 620 nm was observed for 2-(1-carbomethoxy-5-[4-dimethylaminophenyl]-1H-pyrazol-3-yl)phenol in n-heptane and attributed to excited-state intramol. proton transfer. As a result, competitive excited-state proton/charge transfer properties have been observed in the pyrazoles studied, of which the spectral properties can be fine tuned by substituent as well as solvent effects.

IT 246229-49-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and evaluation of excited-state charge transfer and proton transfer in 2-(5-aryl-1-carbomethoxy-1H-pyrazol-3-yl)phenols)

RN 246229-49-2 CAPLUS
CN 1H-Pyrazole-1-carboxylic acid, 3-(2-hydroxyphenyl)-5-(4-methylphenyl)-, methyl ester (9CI) (CA INDEX NAME)



C1 to C8 · R2 = subst. acyl
claim 1

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

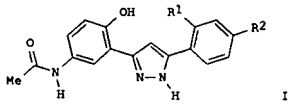
Karen Cheng

10526940species

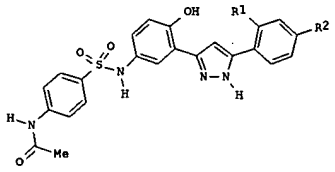
L26 ANSWER 25 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L26 ANSWER 26 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:480956 CAPLUS
DOCUMENT NUMBER: 131:271831
TITLE: Synthesis of some new 3,5-diarylpyrazoles and their antibacterial activity
AUTHOR(S): Palkar, R. B.; Master, H. E.
CORPORATE SOURCE: Nadkarny Sacasa Research Laboratory, Department of Chemistry, St. Xavier's College, Mumbai, 400 001, India
SOURCE: Indian Journal of Heterocyclic Chemistry (1999), 8(4), 315-318
CODEN: IJCHEI; ISSN: 0971-1627
PUBLISHER: Prof. R. S. Varma
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

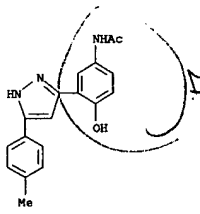
AB 3-(5-Acetamido-2'-hydroxyphenyl)-5-aryl-1H-pyrazoles I (R1 = H, Cl; R2 = H, Me, Cl) were synthesized from 3-(2'-hydroxyphenyl)-5'-aryl-1,3-diketones and 6-acetamidoflavones resp. which on hydrolysis gave the corresponding 5'-amino-2'-hydroxyphenylpyrazole hydrochlorides. Condensation of 5'-amino-2'-hydroxyphenylpyrazole hydrochlorides with p-acetamidobenzenesulfonyl chloride in pyridine gave 3-(5'-acetamidobenzenesulphanilamido-2'-hydroxyphenyl)-5-arylpyrazoles II. I and II have been screened for antimicrobial activity against gram-pos. and gram-neg. bacteria.

IT 245468-37-5P 245468-46-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3,5-diarylpyrazoles and their antibacterial activity)

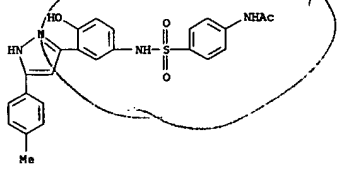
RN 245468-37-5 CAPLUS

L26 ANSWER 26 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CN Acetamide, N-[4-hydroxy-3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]-(9CI) (CA INDEX NAME)



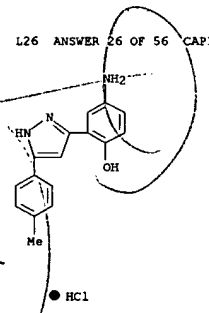
RN 245468-46-6 CAPLUS
CN Acetamide, N-[4-[[[4-hydroxy-3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)



IT 245468-42-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3,5-diarylpyrazoles and their antibacterial activity)

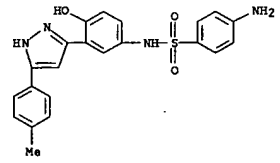
RN 245468-42-2 CAPLUS
CN Phenol, 4-amino-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

L26 ANSWER 26 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 245468-50-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 3,5-diarylpyrazoles and their antibacterial activity)

RN 245468-50-2 CAPLUS
CN Benzenesulfonamide, 4-amino-N-[4-hydroxy-3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Karen Cheng

10526940species

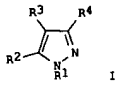
L26 ANSWER 29 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:616374 CAPLUS
DOCUMENT NUMBER: 125:247813
TITLE: Process for preparation of N-substituted pyrazoles.
INVENTOR(S): Merkle, Hans Rupert; Fretschner, Erich; Schroeder, Juergen
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 7 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19509958	A1	19960919	DE 1995-19509958	19950318
CA 2213853	A1	19960912	CA 1996-2213853	19960227
WO 9627589	A1	19960912	WO 1996-EP790	19960227
W: AU, BG, BR, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, PL, SG, SK, TR, UA, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9649418	A	19960923	AU 1996-49418	19960227
AU 698827	B2	19981105		
EP 813526	A1	19971229	EP 1996-905803	19960227
EP 813526	B1	20040204		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL				
CN 1177348	A	19980325	CN 1996-192351	19960227
CN 1070479	B	20010905		
BR 9607649	A	19980616	BR 1996-7649	19960227
HU 9801876	A2	19981130	HU 1998-1876	19960227
HU 221418	B1	20020928		
JP 11501040	T	19990126	JP 1996-526574	19960227
PL 183813	B1	20020731	PL 1996-322114	19960227
AT 258922	T	20040215	AT 1996-905803	19960227
ES 2216045	T3	20041016	ES 1996-905803	19960227
IL 117290	A	20010111	IL 1996-117290	19960228
US 5840913	A	19981124	US 1997-913177	19970820
FI 9703592	A	19970903	FI 1997-3592	19970903
NO 9704044	A	19970903	NO 1997-4044	19970903
NO 307882	B1	20000613		
BG 63304	B1	20010928	BG 1997-101908	19970924

PRIORITY APPLN. INFO.:
DE 1995-19507600 A 19950304
DE 1995-19507699 A 19950304
DE 1995-19509361 A 19950315
DE 1995-19509958 A 19950318
WO 1996-EP790 W 19960227

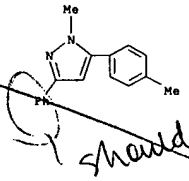
OTHER SOURCE(S): CASREACT 125:247813; MARPAT 125:247813
GI

L26 ANSWER 29 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I

AB N-Substituted pyrazoles I [R1 = C1-12 alkyl, C7-20 phenylalkyl; R2, R3, R4 = H, C1-12, C7-20 alkyl, (un)substituted aryl] are prepared by liquid-phase alkylation of pyrazoles I [R1 = H] with an alc./ester R1OR5 [R1 as above; R5 = H or COR1] at 50-400° and 0.001-100 bar, in the presence of a catalyst. The catalyst can be an acid, alkyl ester, or anhydride, such as H2SO4, Me2SO4, or SO3. For example, reaction of 4-methylpyrazole with MeOH in the presence of H2SO4 at 145° gave 1,4-dimethylpyrazole in 94.4% yield.
IT 66870-43-7P, 1-Methyl-5-(4-methylphenyl)-3-phenylpyrazole
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(product; N-alkylation of pyrazoles with alcs. or esters using acid-type catalysts)
RN 66870-43-7 CAPLUS
CN 1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



should be subst.

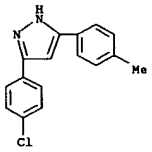
L26 ANSWER 30 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:504142 CAPLUS
DOCUMENT NUMBER: 125:142724
TITLE: Preparation of 3,5-diarylpyrazoles from 1,3-diarylpropenones and hydrazine hydrate in the presence of iodine or iodine compounds and sulfuric acid
INVENTOR(S): Merkle, Hans Rupert; Fretschner, Erich
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 7 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19500838	A1	19960718	DE 1995-19500838	19950113
IN 193044	A1	20040626	IN 1995-MA1718	19951227
CA 2209486	A1	19960718	CA 1996-2209486	19960104
WO 9621650	A1	19960718	WO 1996-EP11	19960104
W: AU, CA, CN, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9644367	A	19960731	AU 1996-44367	19960104
AU 703688	B2	19990401		
EP 802906	A1	19971029	EP 1996-900559	19960104
EP 802906	B1	20051123		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL				
CN 1168136	A	19971217	CN 1996-191420	19960104
CN 1068589	B	20010718		
JP 10511969	T	19981117	JP 1996-521414	19960104
AT 310729	T	20051215	AT 1996-900559	19960104
ES 2255072	T3	20060616	ES 1996-900559	19960104
US 5744614	A	19980428	US 1997-860026	19970703

PRIORITY APPLN. INFO.:
DE 1995-19500838 A 19950113
WO 1996-EP11 W 19960104

OTHER SOURCE(S): CASREACT 125:142724; MARPAT 125:142724
GI

L26 ANSWER 30 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(Preparation)
(prepn. of 3,5-diarylpyrazoles from 1,3-diarylpropenones and hydrazine hydrate in the presence of iodine or iodine compds. and sulfuric acid)
RN 131138-54-0 CAPLUS
CN 1H-Pyrazole, 3-(4-chlorophenyl)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



1025 claims 1-2

103 claim 3

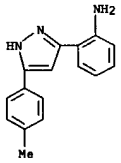
I

AB 3,5-Diarylpyrazoles [I; R1, R3 = (un)substituted aryl; R2 = H, alkyl, (un)substituted aryl] are prepared in high yield by the reaction of hydrazine hydrate, I or I compds., H2SO4, and a 1,3-diarylpropenone R1CH:C(R2)COR3, or by the reaction of hydrazine hydrate, I or I compds., H2SO4, a carbonyl compound R3COCH2R2, and an aryl aldehyde R1CHO. Thus, a mixture of hydrazine hydrate, 4-methylacetophenone, 4-chlorobenzaldehyde, and NaI was dripped into H2SO4, producing 3-(4-chlorophenyl)-5-(4-methylphenyl)pyrazole, m.p. 228°, in 92% theor. yield.
IT 131138-54-0P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP

Karen Cheng

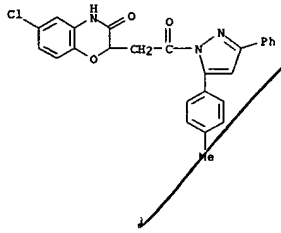
10526940species

L26 ANSWER 31 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:382875 CAPLUS
DOCUMENT NUMBER: 125:75329
TITLE: Synthesis and Binding Activity of Some Pyrazolo[1,5-c]quinazolines as Tools To Verify an Optional Binding Site of a Benzodiazepine Receptor Ligand
AUTHOR(S): Colotta, Vittoria; Catarzi, Daniela; Varano, Flavia; Filacchioni, Guido; Cecchi, Lucia; Galli, Alessandro; Costagli, Chiara
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita' di Firenze, Florence, 50121, Italy
SOURCE: Journal of Medicinal Chemistry (1996), 39(15), 2915-2921
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis and binding activity at the benzodiazepine receptor of some 2-substituted pyrazolo[1,5-c]quinazolines are reported. The structure-activity relationships and in vitro efficacy of the title compds., which are devoid of the proton acceptor atom at position 1, are similar to those of some previously reported tricyclic heteroarom. compds. This suggests that a proton acceptor at position 1 is an optional binding site of a benzodiazepine receptor ligand which only affects potency.
IT 178625-21-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and binding activity of pyrazoloquinazolines as tools to verify
an optional binding site of a benzodiazepine receptor ligand)
RN 178625-21-3 CAPLUS
CN Benzenamine, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

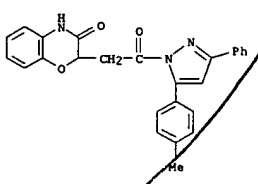


1026 claim 1-2 103 claim 3

L26 ANSWER 32 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



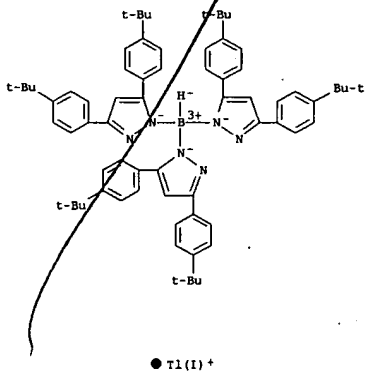
L26 ANSWER 32 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:681195 CAPLUS
DOCUMENT NUMBER: 123:285925
TITLE: Synthesis and biological activities of 1-[(3,4-dihydro-3-oxo-2H-1,4-benzoxazin-2-yl)acetyl]-3,4-disubstituted pyrazoles and 3-methylpyrazoliones
AUTHOR(S): Jayamma, Y.; Reddy, V. Malla
CORPORATE SOURCE: College of Pharmaceutical Sciences, Kakatiya University, Warangal, 506009, India
SOURCE: Indian Journal of Pharmaceutical Sciences (1994), 56(4), 132-5
CODEN: IJSIDW; ISSN: 0250-474X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:285925
AB The title compds., i.e., 2-[2-oxo-2-(oxopyrazol-1-yl)ethyl]-2H-benzoxazin-3(4H)-ones were prepared and tested for their antimicrobial activity.
IT 169760-48-9P 169760-53-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of [oxo(oxopyrazolyl)ethyl]benzoxazinones as antimicrobial agents)
RN 169760-48-9 CAPLUS
CN 1H-Pyrazole, 1-[(3,4-dihydro-3-oxo-2H-1,4-benzoxazin-2-yl)acetyl]-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 169760-53-6 CAPLUS
CN 1H-Pyrazole, 1-[(6-chloro-3,4-dihydro-3-oxo-2H-1,4-benzoxazin-2-yl)acetyl]-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

L26 ANSWER 33 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:93964 CAPLUS
DOCUMENT NUMBER: 120:93964
TITLE: The synthesis of [HB[3,5-(tert-Buph)2pz]3]- (tert-Buph = p-C6H4-tert-Bu), a new tris(pyrazolyl)hydroborato ligand: the crystal and molecular structure of Tl{η3-HB[3,5-(tert-Buph)2pz]3}
AUTHOR(S): Libertini, Emanuela; Yoon, Keum; Parkin, Gerard
CORPORATE SOURCE: Dep. Chem., Columbia Univ., NY, 10027, USA
SOURCE: Polyhedron (1993), 12(20), 2539-43
CODEN: PLYHDE; ISSN: 0277-5387
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of a new sterically demanding tris(pyrazolyl)hydroborato ligand, [HB[3,5-(tert-Buph)2pz]3]- (tert-Buph = p-C6H4(CMe3)), is reported. The K derivative is prepared by the direct reaction of KBH4 with 3,5-bis(p-tert-butylphenyl)pyrazole. Metathesis with TlNO3 converts the K derivative to the Tl complex Tl{η3-HB[3,5-(tert-Buph)2pz]3}. The crystal and mol. structures of the pyrazole derivative [3,5-(tert-Buph)2pz]2ZnI2 and the Tl derivative Tl{η3-HB[3,5-(tert-Buph)2pz]3} were determined
IT 152692-47-2P 152728-23-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
RN 152692-47-2 CAPLUS
CN Borate(1-), tris[3,5-bis[4-(1,1-dimethylethyl)phenyl]-1H-pyrazolato-N1]hydro-, thallium(1+), (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

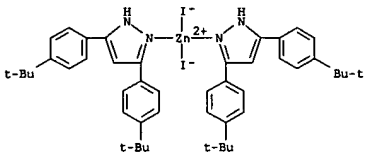
● Tl(I)+

RN 152728-23-9 CAPLUS
CN Zinc, bis[3,5-bis[4-(1,1-dimethylethyl)phenyl]-1H-pyrazole-N2]diiodo-, (T-4)- (9CI) (CA INDEX NAME)

Karen Cheng

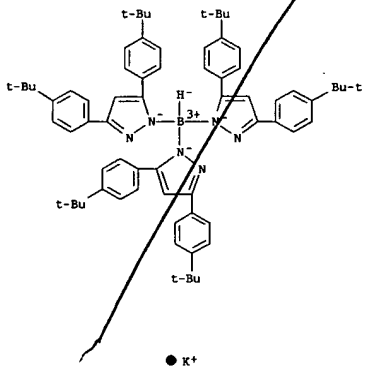
10526940species

L26 ANSWER 33 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 152692-46-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and metathesis of, with thallium nitrate)
RN 152692-46-1 CAPLUS
CN Borate(1-), tris[3,5-bis[4-(1,1-dimethylethyl)phenyl]-1H-pyrazolato-N1]hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A

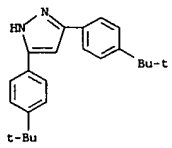


PAGE 2-A

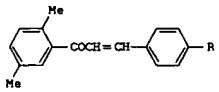
● K+

IT 152503-09-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

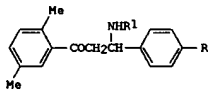
L26 ANSWER 33 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(Reactant or reagent)
(prepn. and reaction of, with potassium borohydride)
RN 152503-09-8 CAPLUS
CN 1H-Pyrazole, 3,5-bis[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



L26 ANSWER 34 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:212582 CAPLUS
DOCUMENT NUMBER: 118:212582
TITLE: Synthesis and some reactions of benzylidene acetophenone derivatives
AUTHOR(S): El-Bahaie, S.; Bayoumy, B. E.; El-Mobayed, M.; Abd El-Latif, G.
CORPORATE SOURCE: Fac. Sci., Zagazig Univ., Zagazig, Egypt
SOURCE: Egyptian Journal of Chemistry (1991), Volume Date 1990, 33(5), 429-38
CODEN: EGJCA3; ISSN: 0367-0422
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

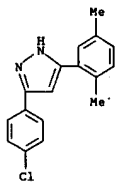


I



II

AB Benzylideneacetophenones I (R = Cl, NO2) react are epoxidized to give the corresponding oxiranes. Amination of I with R1NH2 (R1 = CH2Ph, 4-MeOC6H4) gave aminated derivs. II. I and other derivs. of I underwent various other reactions.
IT 146529-43-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 146529-43-3 CAPLUS
CN 1H-Pyrazole, 3-(4-chlorophenyl)-5-(2,5-dimethylphenyl)- (9CI) (CA INDEX NAME)



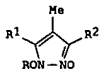
L26 ANSWER 34 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

1026 Claim 1-2
103 claim 3

Karen Cheng

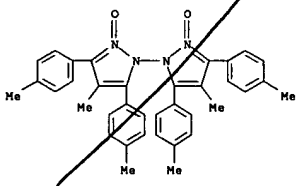
10526940species

L26 ANSWER 35 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:633220 CAPLUS
DOCUMENT NUMBER: 117:233220
TITLE: Degenerate and nondegenerate reversible [1,7] O .dblharw. O' alkylotropy of 1-hydroxypyrazole 2-oxides. Variation of channels of associated molecular rearrangements
AUTHOR(S): Olekhnovich, L. P.; Tkachuk, A. V.; Budarina, Z. N.; Ivakhnenko, E. P.; Tseimakh, I. D.; Knyazev, A. P.; Zhdanov, Yu. A.
CORPORATE SOURCE: Rostov. Gos. Univ., Rostov, USSR
SOURCE: Doklady Akademii Nauk SSSR (1991), 321(3), 530-7 [Chem.]
CODEN: DANKAS; ISSN: 0002-3264
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 117:233220
GI



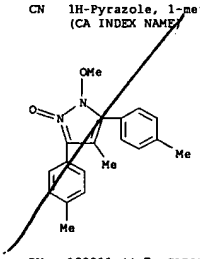
I

AB Rearrangements in alkoxypyrazole oxides I (R = Me, PhCH2; R1, R2 = Ph, p-tolyl, Me) occurred by [1,7]-O .dblharw. O' shift of R, [1,5]-N → C and/or [1,3]-N → C shift of RO, and, in the case of R = PhCH2, homolytic N-O bond cleavage. Kinetic data were obtained.
IT 139911-54-9P
RL: PREP (Preparation)
(formation and dissociation of, kinetics of)
RN 139911-54-9 CAPLUS
CN 1,1'-Bi-1H-pyrazole, 4,4'-dimethyl-3,3',5,5'-tetrakis(4-methylphenyl)-, 2,2'-dioxide (9CI) (CA INDEX NAME)

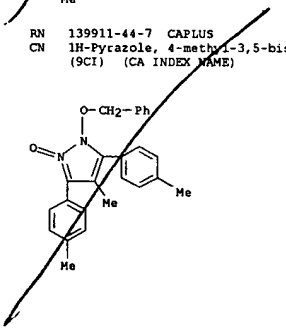


IT 139911-42-5 139911-44-7
RL: RCT (Reactant); RACT (Reactant or reagent)

L26 ANSWER 35 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(rearrangement of, kinetics and mechanism of)
RN 139911-42-5 CAPLUS
CN 1H-Pyrazole, 1-methoxy-4-methyl-3,5-bis(4-methylphenyl)-, 2-oxide (9CI) (CA INDEX NAME)



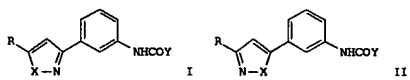
RN 139911-44-7 CAPLUS
CN 1H-Pyrazole, 4-methyl-3,5-bis(4-methylphenyl)-1-(phenylmethoxy)-, 2-oxide (9CI) (CA INDEX NAME)



L26 ANSWER 36 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:171439 CAPLUS
DOCUMENT NUMBER: 117:171439
TITLE: Preparation of 3-[3(5)-pyrazolyl or isoxazolyl]aniline derivatives and herbicides containing them
INVENTOR(S): Koyanagi, Hiroshi; Nishisaka, Takashi; Yoshida, Shigeo
PATENT ASSIGNEE(S): SDS Biotech K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04124178	A	19920424	JP 1990-241616	19900912
PRIORITY APPLN. INFO.:			JP 1990-241616	19900912

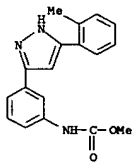
OTHER SOURCE(S): MARPAT 117:171439
GI



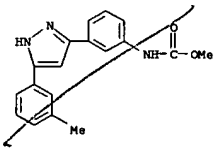
I II

AB The title derivs. I [R = lower alkyl, (un)substituted Ph; X = NH, NMe, O; Y = lower alkyl, lower alkenyl, lower alkoxy, lower alkenyloxy, N,N-dialkylamino, N-lower alkyl-N-lower alkoxyamino] or II and herbicides containing I or II are claimed. ClCO2Me was added dropwise to 3-tert-butyl-5-(3-aminophenyl)pyrazole (prepared by reduction of the corresponding nitro compound) in pyridine at 0° and the reaction mixture was further stirred at room temperature for 5 h to give 90% I (R = CMe3, X = NH, Y = OMe) (III). III at 4 kg active ingredient/ha completely controlled barnyard grass, Scirpus juncoides, Monochoria vaginalis, and Ammannia multiflora grown on paddy filed without any damage to rice plant.
IT 143704-56-7P 143704-57-8P 143704-58-9P
143704-59-0P 143704-60-3P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)
RN 143704-56-7 CAPLUS
CN Carbamic acid, [3-[5-(2-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

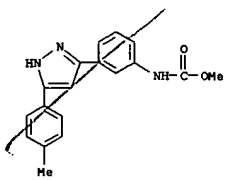
L26 ANSWER 36 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 143704-57-8 CAPLUS
CN Carbamic acid, [3-[5-(3-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 143704-58-9 CAPLUS
CN Carbamic acid, [3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 143704-59-0 CAPLUS
CN Carbamic acid, [3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

okay
1026claim 1-2
103 claim 3

Karen Cheng

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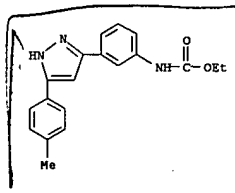
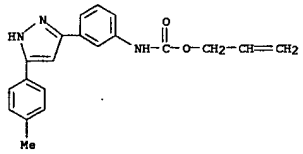
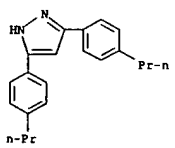
L26 ANSWER 36 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 143704-60-3 CAPLUS
CN Carbamic acid, [3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, 2-propenyl ester (9CI) (CA INDEX NAME)

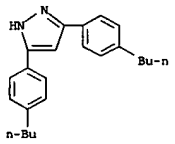


L26 ANSWER 37 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:561422 CAPLUS
DOCUMENT NUMBER: 117:161422
TITLE: Synthesis and mesomorphic properties of the 3,5-bis-alkoxyphenyl-pyrazoles and -isoxazoles
AUTHOR(S): Bartulin, J.; Martinez, R.; Mueller, H. J.; Fan, Z. X.; Haase, W.
CORPORATE SOURCE: Fac. Cienc., Univ. Concepcion, Chile
SOURCE: Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1992), 220, 67-75
CODEN: MCLCE9; ISSN: 1058-725X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis and measurement of phys. properties using DSC, x-ray and optical methods are described for the 3,5-bis(p-alkoxyphenyl)pyrazole and 3,5-bis(p-alkoxyphenyl)isoxazole series with the C number of the alkyl group from 3 to 8. The pyrazole series with longer alkyl groups (6, 7, and 8) show the smectic A as well as smectic C phases. The corresponding isoxazole compds. show nematic and also smectic A phases. The compds. with shorter alkyl groups (3, 4 and 5) show either nematic or smectic A phases for both series, resp.
IT 143613-60-9P 143613-61-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and liquid crystal properties of)
RN 143613-60-9 CAPLUS
CN 1H-Pyrazole, 3,5-bis(4-propylphenyl)- (9CI) (CA INDEX NAME)



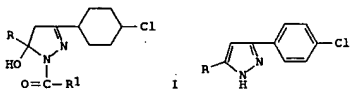
1026 = 142
103 = 3

RN 143613-61-0 CAPLUS
CN 1H-Pyrazole, 3,5-bis(4-butylphenyl)- (9CI) (CA INDEX NAME)

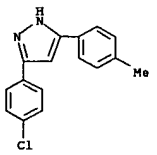


L26 ANSWER 37 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L26 ANSWER 38 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:23863 CAPLUS
DOCUMENT NUMBER: 114:23863
TITLE: Reactions of aroylhydrazines with chalcone dibromides
AUTHOR(S): Holla, B. Shivarama; Udupa, K. Venkatramana
CORPORATE SOURCE: Dep. P G Stud. Res. Chem., Mangalore Univ., Mangalagangothri, 574 199, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1990), 29B(9), 887-9
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:23863
GI



AB Cyclization of p-ClC6H4CH(Br)CH(Br)C(O)R (R = Ph, p-tolyl, p-ClC6H4) with R1C(O)NHNH2 (R1 = Ph, o-, p-ClC6H4, p-HOC6H4, 2-naphthyloxymethyl) gave 60-9% 13 pyrazolines I, which underwent acid catalyzed dehydration to give 75-80% pyrazoles II.
IT 131138-54-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 131138-54-0 CAPLUS
CN 1H-Pyrazole, 3-(4-chlorophenyl)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



1026 = 142
103 = 3

Karen Cheng

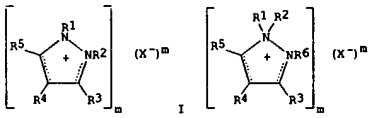
10526940species

103 art.

L26 ANSWER 42 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:16078 CAPLUS
DOCUMENT NUMBER: 96:16078
TITLE: Composition containing a pyrazolium salt for retarding the growth of sunflower
INVENTOR(S): Shafer, Neal E.; Bhalla, Prithvi Raj
PATENT ASSIGNEE(S): American Cyanamid Co. , USA
SOURCE: Fr. Demande, 28 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2475853	A1	19810821	FR 1981-3167	19810218
CA 1151890	A1	19830816	CA 1981-369468	19810128
BR 8100964	A	19810825	BR 1981-964	19810218
AU 8167409	A	19810827	AU 1981-67409	19810218
ZA 8101086	A	19820331	ZA 1981-1086	19810218
ES 499545	A1	19820901	ES 1981-499545	19810218
HU 27555	A2	19831028	HU 1981-390	19810218

PRIORITY APPLN. INFO.: US 1980-122642 A 19800219
GI



I II

AB The pyrazolium salts I or II (R1 and R2 C1-3 alkyl or Ph; R4 = H, OH, C1-18 alkyl, haloalkyl, alkoxy, PhCH2, substituted Ph, etc.; R3 and R5 = C1-12 alkyl, alkoxy, cycloalkyl, halo, NH2, PhNH, EtO, naphthyloxy, heterocyclic radical, etc.; R6 = H or Me; X = acetate, sulfate, etc.; m = 1, 2, or 3) are growth inhibitors for sunflower. Thus, preplant 1,2-dimethyl-3,5-diphenylpyrazolium Me sulfate [43222-48-6] (0.25 kg/ha) decreased the height of sunflower by 69.6%.
IT 43222-79-3 58538-73-1
RL: BIOL (Biological study)
(plant growth inhibitor, for sunflower)
RN 43222-79-3 CAPLUS
CN 1H-Pyrazolium, 1,2-dimethyl-3,5-bis(4-methylphenyl)-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

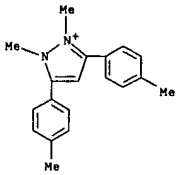
CRN 49867-86-9
CMF C19 H21 N2

L26 ANSWER 42 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 21228-90-0
CMF C H3 O4 S

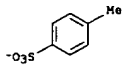
Me-O-SO3-

L26 ANSWER 42 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

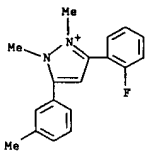
CRN 16722-51-3
CMF C7 H7 O3 S



RN 58538-73-1 CAPLUS
CN 1H-Pyrazolium, 3-(2-fluorophenyl)-1,2-dimethyl-5-(3-methylphenyl)-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 58538-72-0
CMF C18 H18 F N2

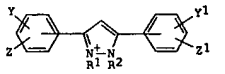


CM 2

L26 ANSWER 43 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:17174 CAPLUS
DOCUMENT NUMBER: 92:17174
TITLE: Herbicidal combinations
INVENTOR(S): Feeny, Richard W.
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: U.S., 13 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

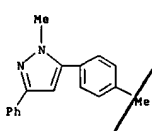
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4170464	A	19791009	US 1977-822504	19770808
US 3867403	A	19750218	US 1972-307670	19721117
			US 1972-307670	A3 19721117
			US 1974-518020	A2 19741025

PRIORITY APPLN. INFO.:
GI



I

AB Mixts. of 1,2-dialkyl-3,5-diphenylpyrazolium salts and chlorophenoxyalkanoates or the diphenylpyrazolium chlorophenoxyalkanoates I (R1 and R2 = alkyl; R3 = Cl or Me; R4 = H or Me; Y, Y1, Z, Z1 = H, halo, Me, or MeO) are synergistic herbicides. Thus, a composition containing 1,2-dimethyl-3,5-diphenylpyrazolium Me sulfate [43222-48-6] (1.12 kg/ha) and 2,4-D dimethylamine salt [2008-39-1] (0.56 kg/ha) almost totally controlled pepperweed, pennycress, and shepherd's purse, with min. phytotoxicity to winter wheat, whereas the pyrazolium compound by itself showed little herbicidal activity.
IT 66870-43-7P 72218-38-3P 72218-42-9P
72218-43-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkylation of)
RN 66870-43-7 CAPLUS
CN 1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 72218-38-3 CAPLUS
CN 1H-Pyrazole, 5-(2,6-dimethylphenyl)-1-methyl-3-phenyl- (9CI) (CA INDEX

Wt. 9
Sub.

Karen Cheng

10526940species

L26 ANSWER 46 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:433005 CAPLUS
DOCUMENT NUMBER: 85:33005
TITLE: Pyrazole plant growth regulants
INVENTOR(S): Johnson, Alexander Lawrence; Sweetser, Philip B.
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA
SOURCE: U.S., 15 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

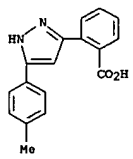
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3948937	A	19760406	US 1973-397720	19730917
IL 39092	A	19760229	IL 1972-39092	19720327
IT 955155	B	19730929	IT 1972-22831	19720407
AU 7241026	A	19731018	AU 1972-41026	19720412
ZA 7202576	A	19730131	ZA 1972-2576	19720417
ES 401879	A1	19760201	ES 1972-401879	19720418
CA 982588	A1	19760127	CA 1972-140051	19720419
BR 7202417	D0	19730503	BR 1972-2417	19720420
NL 7205441	A	19721024	NL 1972-5441	19720421
FR 2136595	A5	19721222	FR 1972-14198	19720421
JP 58011401	B	19830302	JP 1972-39729	19720421
US 4055409	A	19771025	US 1975-627462	19751030
PRIORITY APPLN. INFO.:			US 1971-136576 A2	19710422
			US 1972-230508 A2	19720229
			US 1973-397720 A3	19730917

GI

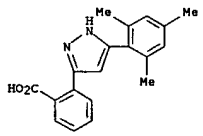
I

AB Pyrazoles (I, R = 2-HO2CC6H4, substituted 2-carboxyphenyl; R1 = Ph, substituted phenyl) (35 compds.) were prepared Thus, 100 g di-Na salt of 2-benzoylacetylbenzoic acid in MeOH-HCl was cyclized with 11 g NH2NH2 to give 59 g of I (R = 2-HO2CC6H4, R1 = Ph). I at low rates, 0.001 - 4 lb/acre, are plant growth regulators and at higher rates, 0.5-10 lb/acre, exhibit herbicidal activity.
IT 39784-92-4P 39784-96-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 39784-92-4 CAPLUS
CN Benzoic acid, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L26 ANSWER 46 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

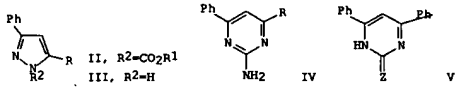


RN 39784-96-8 CAPLUS
CN Benzoic acid, 2-[5-(2,4,6-trimethylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



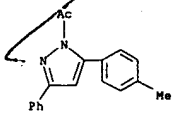
1026 = 1, 2
103 = 3

L26 ANSWER 47 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:432950 CAPLUS
DOCUMENT NUMBER: 85:32950
TITLE: Acetylinic ketones. Part II. Reaction of acetylenic ketones with nucleophilic nitrogen compounds
AUTHOR(S): Baddar, F. G.; Al-Hajjar, F. H.; El-Rayyes, N. R.
CORPORATE SOURCE: Dep. Chem., Kuwait Univ., Kuwait, Kuwait
SOURCE: Journal of Heterocyclic Chemistry (1976), 13(2), 257-68
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 85:32950
GI

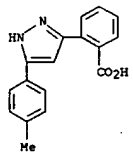


II, R^2=CO_2R^1 III, R^2=H IV V

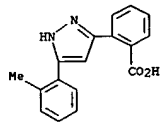
AB PhC.tplbond.CCOR [I, R = Ph, C6H4Me-p, C6H4Cl-m, p, C6H4OMe-p, 3,4-(methylenedioxy)phenyl] reacted with H2NNHCO2R1 (R1 = Ph, Et) to give RCOCH:CPhNHNHCO2R1, which were cyclized with Ac2O to give the pyrazolecarboxylates II, which on hydrolysis-decarboxylation with MeOH-NaOH gave the aromatic pyrazoles III; I also reacted with NH2C(:NH)NH2 to give the pyrimidines IV; similarly, the pyrimidines V (Z = S, O) were prepared from heating PhC.tplbond.CCOPh with H2NC(:Z)NH2.
IT 59807-09-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 59807-09-9 CAPLUS
CN 1H-Pyrazole, 1-acetyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



L26 ANSWER 48 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:131323 CAPLUS
DOCUMENT NUMBER: 84:131323
TITLE: Effect of substituted pyrazoles and related compounds on geotropism in cress seedlings
AUTHOR(S): Geissler, Alt E.; Huppatz, John L.; Katekar, Gerard F.
CORPORATE SOURCE: Div. Plant Ind., CSIRO, Canberra, Australia
SOURCE: Pesticide Science (1975), 6(5), 441-50
CODEN: PSSCBG; ISSN: 0031-613X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 2-Phenyl-8H-pyrazolo[5,1-a]isoindol-8-one (I) [37564-20-8], 5-(2-carboxyphenyl)-3-phenylpyrazole [39784-88-8], and derivs. of both these compds. were highly active against root geotropism in cress seedling, destruction of geotropism occurring at 10-7-10-9M. Substitution with functional groups and increased mol. size caused only minor variations in activity.
IT 39784-92-4P 58726-52-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and geotropic activity of)
RN 39784-92-4 CAPLUS
CN Benzoic acid, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 58726-52-6 CAPLUS
CN Benzoic acid, 2-[5-(2-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



Karen Cheng

10526940species

L26 ANSWER 49 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

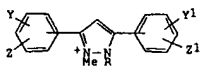
ACCESSION NUMBER: 1976:116915 CAPLUS
DOCUMENT NUMBER: 84:116915
TITLE: Pyrazolium fungicides
INVENTOR(S): Walworth, Bryant L.
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 7
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3930011	A	19751230	US 1975-546654	19750203
ZA 7507951	A	19761229	ZA 1975-7951	19751222
IL 48708	A	19780731	IL 1975-48708	19751223
AU 7587903	A	19770630	AU 1975-87903	19751224
AU 500653	B2	19790531		
GB 1534866	A	19781206	GB 1975-53214	19751230
CA 1058517	A1	19790717	CA 1976-243287	19760109
NL 7600700	A	19760805	NL 1976-700	19760123
DK 7600296	A	19760804	DK 1976-296	19760126
DK 139833	C	19791001		
DK 139833	B	19790430		
FI 7600174	A	19760804	FI 1976-174	19760126
FI 59194	B	19810331		
FI 59194	C	19810710		
DE 2602964	A1	19760805	DE 1976-2602964	19760127
CS 199651	B2	19800731	CS 1976-580	19760129
BE 838171	A4	19760802	BE 1976-164007	19760202
SE 7601095	A	19760803	SE 1976-1095	19760202
SE 420888	B	19811109		
SE 420888	C	19820218		
NO 7600343	A	19760804	NO 1976-343	19760202
NO 145039	B	19810921		
NO 145039	C	19820104		
BR 7600646	A	19760831	BR 1976-646	19760202
CH 594354	A5	19780113	CH 1976-1243	19760202
AT 347178	B	19781211	AT 1976-697	19760202
SU 644359	A3	19790125	SU 1976-2319208	19760202
FR 2298949	A2	19760827	FR 1976-2975	19760203
FR 2298949	B2	19790330		
JP 51104031	A	19760914	JP 1976-10777	19760203
DD 124703	A6	19770309	DD 1976-191070	19760203

PRIORITY APPLN. INFO.:
US 1971-209448 A 19711217
US 1972-271424 A 19720713
GB 1972-55680 A 19721201
US 1975-546654 A 19750203

GI

L26 ANSWER 49 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I

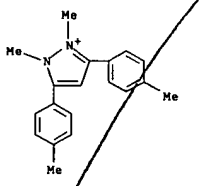
AB Dialkyldiphenylpyrazolium salts I (R=alkyl, allyl, propynyl, ethylcarboxymethyl, Ph, or PhCH2; Y,Y',Z, and Z'=H, halogen, C1-4 alkyl or alkoxy; X=mono- or divalent anion; m = 1 or 2) were effective as fungicides. For example, 1,2-dimethyl-3,5-diphenylpyrazolium methyl sulfate [43222-48-6] was effective for control of Phytophthora infestans on tomato, Piricularia oryzae on rice, and Venturia inaequalis on apple. The synthesis of I is described.

IT 43222-60-2P 43222-78-2P 43222-79-3P
58538-18-4P 58538-19-5P 58538-21-9P
58538-22-0P 58538-34-4P 58538-37-7P
58538-38-8P 58538-47-9P 58538-59-3P
58538-67-3P 58538-68-4P 58538-73-1P
58538-74-2P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and fungicidal activity of)

RN 43222-60-2 CAPLUS
CN 1H-Pyrazolium, 1,2-dimethyl-3,5-bis(4-methylphenyl)-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 49867-86-9
CMF C19 H21 N2



CM 2

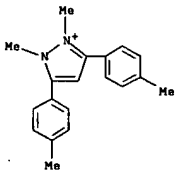
CRN 14797-73-0
CMF Cl O4

L26 ANSWER 49 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 43222-78-2 CAPLUS
CN 1H-Pyrazolium, 1,2-dimethyl-3,5-bis(4-methylphenyl)-, methyl sulfate (9CI) (CA INDEX NAME)

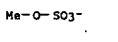
CM 1

CRN 49867-86-9
CMF C19 H21 N2



CM 2

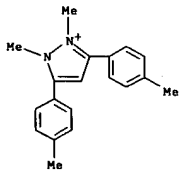
CRN 21228-90-0
CMF C H3 O4 S



RN 43222-79-3 CAPLUS
CN 1H-Pyrazolium, 1,2-dimethyl-3,5-bis(4-methylphenyl)-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

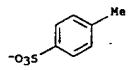
CM 1

CRN 49867-86-9
CMF C19 H21 N2



CM 2

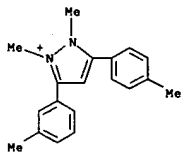
CRN 16722-51-3
CMF C7 H7 O3 S



RN 58538-18-4 CAPLUS
CN 1H-Pyrazolium, 1,2-dimethyl-3-(3-methylphenyl)-5-(4-methylphenyl)-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 58538-17-3
CMF C19 H21 N2



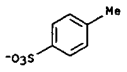
CM 2

CRN 21228-90-0
CMF C H3 O4 S

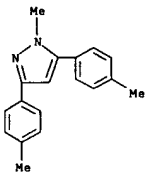
Karen Cheng

10526940species

L26 ANSWER 52 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 43222-89-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization of)
RN 43222-89-5 CAPLUS
CN 1H-Pyrazole, 1-methyl-3,5-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

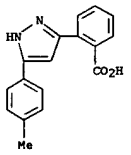


L26 ANSWER 53 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:58410 CAPLUS
DOCUMENT NUMBER: 78:58410
TITLE: Plant growth regulating 3,5-diphenylpyrazoles
INVENTOR(S): Johnson, Alexander Lawrence; Sweetser, Philip Bliss
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co.
SOURCE: Ger. Offen., 70 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2219702	A	19721116	DE 1972-2219702	19720421
IL 39092	A	19760229	IL 1972-39092	19720327
IT 955155	B	19730929	IT 1972-22831	19720407
AU 7241026	A	19731018	AU 1972-41026	19720412
ZA 7202576	A	19730131	ZA 1972-2576	19720417
ES 401879	A1	19760201	ES 1972-401879	19720418
CA 982588	A1	19760127	CA 1972-140051	19720419
BR 7202417	D0	19730503	BR 1972-2417	19720420
NL 7205441	A	19721024	NL 1972-5441	19720421
FR 2136595	A5	19721222	FR 1972-14198	19720421
JP 58011401	B	19830302	JP 1972-39729	19720421
PRIORITY APPLN. INFO.:			US 1971-136576 A	19710422
			US 1972-230508 A	19720229

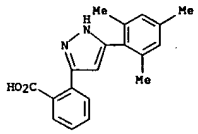
GI For diagram(s), see printed CA Issue.
AB About 30 title compds. (e.g. I, Rn = 4-F, 3-MeO, 4-Me, 3-Br, 2,4,6-Me3, 4-Cl, or 2-MeO; R1 = H or Et; R2 = H, Me, or Ac; R3 = OH, OMe, OEt, OPr, OBu, OCH2CH2OH, COSH, CONH2, or CONHBu; R4 = H or Me) were prepared either from phthalic anhydride (or its 4-methyl derivative) and MeCOC6H5-nRn via 2,4-NaO2CR4C6H3COCHNaCOC6H5-nRn and reaction with R2NHNH2 or (in the case of R1 = R2 = R4 = H) by cleavage of II with R3H and optionally Na. I were used against weeds in culture plant fields, e.g. sugar cane, soybean, peanut, or citrus, and for growth regulation of cotton, soybeans, and peanuts.
IT 39784-92-4P 39784-96-8P 39785-13-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 39784-92-4 CAPLUS
CN Benzoic acid, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L26 ANSWER 53 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

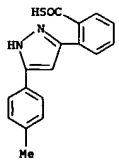


1026 = 1-2
103-3.

RN 39784-96-8 CAPLUS
CN Benzoic acid, 2-[5-(2,4,6-trimethylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



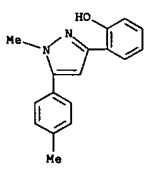
RN 39785-13-2 CAPLUS
CN Benzenecarbothioic acid, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



L26 ANSWER 54 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:564690 CAPLUS
DOCUMENT NUMBER: 77:164690
TITLE: Pharmacologically active 5-(o-hydroxyphenyl)pyrazoles
PATENT ASSIGNEE(S): Ferlux
SOURCE: Fr. Demande, 22 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2104932	A1	19720428	FR 1970-32535	19700908
FR 2104932	A5	19720428		
FR 2104932	B1	19740830		
PRIORITY APPLN. INFO.:			FR 1970-32535 A	19700908

GI For diagram(s), see printed CA Issue.
AB 5-(o-Hydroxyphenyl)pyrazoles I (R = 2-FC6H4, 4-FC6H4, 3,4-C12C6-H3, 3,4-(MeO)2C6H3, 4-MeC6H4, 4-(O2N)C6H4, 3-ClC6H4, Ph, 2-furyl; R1 = H, Me, Ph, p-(O2N)C6H4, PhCH2CH2) were prepared Thus treatment of o-HOC6H4COMe with o-FC6H4COCl gave 2-(o-FC6H4CO2)C6H4COMe, which on treatment with K in pyridine gave the K salt of o-HOC6H4COCH2COC6H4F-o. The latter was cyclized with MeNHNH2 to I (R = o-FC6H4, R1 = Me). I showed antiinflammatory, analgesic, sedative, diuretic, and hypocholesteremic activity in a variety of tests.
IT 38371-76-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38371-76-5 CAPLUS
CN Phenol, 2-[1-methyl-5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

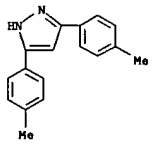


1026 - claim 1-3
claim 9?

Karen Cheng

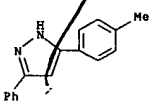
10526940species

L26 ANSWER 55 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:3172 CAPLUS
DOCUMENT NUMBER: 60:3172
ORIGINAL REFERENCE NO.: 60:527b-c
TITLE: Extrusion of sulfur. VI. Novel ring-contractions giving pyridazines and pyrazoles
AUTHOR(S): London, J. D.; Young, L. B.
CORPORATE SOURCE: Univ. Glasgow, UK
SOURCE: Journal of the Chemical Society (1963), (Nov.), 5496-5502
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 60:3172
GI For diagram(s), see printed CA Issue.
AB cf. CA 57, 12434f. 2,7-Dihydro-3,6-diphenyl-1,4,5thiadiazepine (I) yields 3,6-diphenylpyridazine (II) by halogenation-dehalogenation or by thermal decomposition When heated in acetic acid its S,S-dioxide also yields the pyridazine, whereas its S-monoxide affords 3,5-diphenylpyrazole (III) and hence, in presence of H2O2, 2,5-diphenyl-1,3,4-oxadiazole (IV) and 1,2-dibenzoylhydrazine. The S,S-dioxide is isomerized by NaOEt-EtOH to a sulfinic acid which loses SO2 when melted and yields 3-methyl-4,5-diphenylpyrazole (V).
IT 93330-77-9P, Pyrazole, 3,5-di-p-tolyl-
RL: PREP (Preparation)
(preparation of)
RN 93330-77-9 CAPLUS
CN 1H-Pyrazole, 3,5-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)



1026-1-2
103=B

L26 ANSWER 56 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1939:11351 CAPLUS
DOCUMENT NUMBER: 33:11351
ORIGINAL REFERENCE NO.: 33:1727d-g
TITLE: Reactions of phenylpropiol-4-iodoanilide and similar thioamides
AUTHOR(S): Worrall, David E.; Lerner, Morris; Washnock, John, Jr.
SOURCE: Journal of the American Chemical Society (1939), 61, 105-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The thioamides were prepared from PhC.tbond.CNa and the appropriate isothiocyanate in Et2O in 60-80% yields; all but the 4-Ph derivative (bright yellow) were pale yellow; the substances were polymerized by heating Et2O solns. containing a little NaOH; these are brown or greenish brown and melt with decomposition Aniline-substituted phenylpropiolthioanilides: 4-I, m. 140-1° (dimer, m. above 173°); 4-EtO, m. 111-12° (dimer, m. 199-200°); 3-Br, m. 100-1° (dimer, indefinite m. p.); 4-Ph, m. 128-9° (dimer, m. 230-2°); α-naphthyl, m. 104-5°. NH2OH gives 5-phenylisoxazoles in 20-30% yields; 3-(4-iodoanilino), m. 148-9°; 4-Br derivative, m. 172-3°; 4-Cl derivative, m. 151-2°; 4-NO2 derivative, m. 243-4°; 3-(2-bromo-p-toluidino)-4-bromo, m. 130-1°; 3-(2,6-dichloro-p-toluidino)-4-chloro, m. 229-30°; 3-(4-phenylanilino), m. 176-7°. 5-Phenylpyrazoles; 3-(4-iodoanilino), m. 175-6°; 3-(2-bromo-4-iodoanilino)-4-bromo, m. 201-2°; 3-(4-iodoanilino)-4-chloro, m. 206-7°; 3-(3-bromoanilino), m. 205-6°; 3-(3-bromoanilino)-4-bromo, m. 178-9°; 3-(p-toluidino), m. 157-8°; 3-(2-bromo-p-toluidino)-4-bromo, m. 181-2°; 3-(2,6-dinitro-p-toluidino)-4-nitro, m. 245-7°; 3-(4-phenylanilino), m. 219-20°.
IT 854699-53-9P, Pyrazole, 3-phenyl-5-p-toluino-
RL: PREP (Preparation)
(preparation of)
RN 854699-53-9 CAPLUS
CN Pyrazole, 3-phenyl-5-p-toluino- (4CI) (CA INDEX NAME)



Karen Cheng

10526940claim4

search claim4

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8
NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:14:23 ON 01 MAR 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:14:32 ON 01 MAR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1
DICTIONARY FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

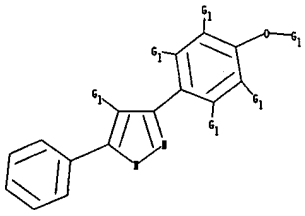
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

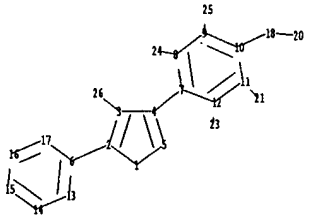
http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10526940claim4.str

Karen Cheng

10526940claim4





chain nodes :
18 20 21 23 24 25 26
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
2-6 3-26 4-7 8-24 9-25 10-18 11-21 12-23 18-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14
14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 3-26 4-5 8-24 9-25 10-18 11-21 12-23 18-20
exact bonds :
2-3 2-6 3-4 4-7
normalized bonds :
6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 6 : 7 :

G1:H,CH3

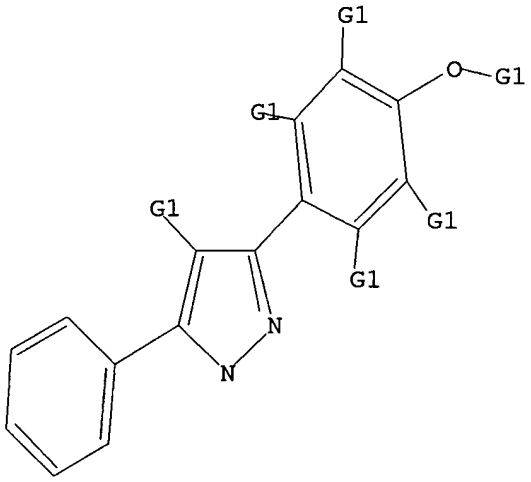
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS
21:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

L1 STRUCTURE UPLOADED

Karen Cheng

10526940claim4

=> d
L1 HAS NO ANSWERS
L1 STR



G1 H,Me

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 17:14:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 106151 TO ITERATE

100.0% PROCESSED 106151 ITERATIONS 854 ANSWERS
SEARCH TIME: 00.00.01

L2 854 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 17:14:57 ON 01 MAR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 1 Mar 2007 VOL 146 ISS 10

Karen Cheng

10526940claim4

FILE LAST UPDATED: 28 Feb 2007 (20070228/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

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=> s l2
L3 155 L2

=> d ibib abs hitstr 120-155

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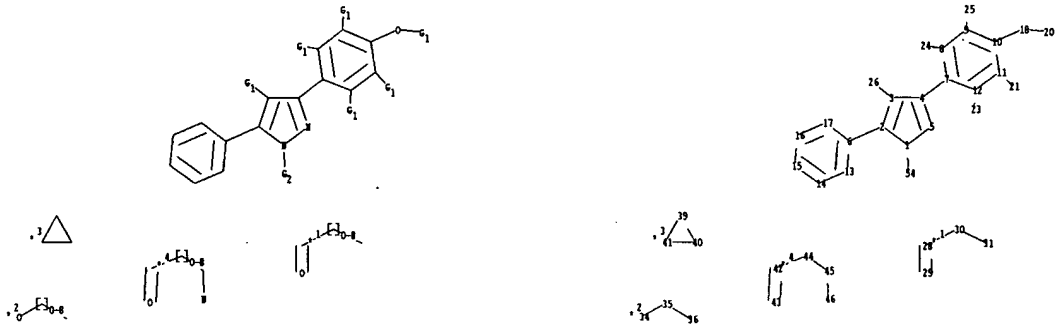
10526940claim4

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10526940cla4.str



chain nodes :
18 20 21 23 24 25 26 28 29 30 31 34 35 36 42 43 44 45 46 54
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 39 40 41
chain bonds :
1-54 2-6 3-26 4-7 8-24 9-25 10-18 11-21 12-23 18-20 28-30 28-29 30-31
34-35 35-36 42-43 42-44 44-45 45-46
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14
14-15 15-16 16-17 39-40 39-41 40-41
exact/norm bonds :
1-2 1-5 1-54 3-26 4-5 8-24 9-25 10-18 11-21 12-23 18-20 28-29 34-35
42-43 45-46
exact bonds :
2-3 2-6 3-4 4-7 28-30 30-31 35-36 39-40 39-41 40-41 42-44 44-45
normalized bonds :
6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 6 : 7 : 39 :

G1:H,CH3

G2:H,Ak,[*1],[*2],[*3],[*4]

Karen Cheng

10526940claim4

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS
21:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 34:CLASS 35:CLASS 36:CLASS 39:Atom 40:Atom 41:Atom 42:CLASS
43:CLASS 44:CLASS 45:CLASS 46:CLASS 54:CLASS

L6 STRUCTURE UPLOADED

=> d
L6 HAS NO ANSWERS
L6 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> d his

(FILE 'HOME' ENTERED AT 17:14:23 ON 01 MAR 2007)

FILE 'REGISTRY' ENTERED AT 17:14:32 ON 01 MAR 2007
L1 STRUCTURE UPLOADED
L2 854 S L1 FULL

FILE 'CAPLUS' ENTERED AT 17:14:57 ON 01 MAR 2007
L3 155 S L2

FILE 'REGISTRY' ENTERED AT 17:16:13 ON 01 MAR 2007
L4 STRUCTURE UPLOADED
L5 671 S L4 FULL SUB=L2

FILE 'STNGUIDE' ENTERED AT 17:16:48 ON 01 MAR 2007

FILE 'REGISTRY' ENTERED AT 17:20:20 ON 01 MAR 2007
L6 STRUCTURE UPLOADED

=> s l6 full sub=l2
FULL SUBSET SEARCH INITIATED 17:20:48 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 854 TO ITERATE

100.0% PROCESSED 854 ITERATIONS 165 ANSWERS
SEARCH TIME: 00.00.01

L7 165 SEA SUB=L2 SSS FUL L6

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 41.10 445.53

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

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10526940claim4

	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-28.08

FILE 'CAPLUS' ENTERED AT 17:20:51 ON 01 MAR 2007
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FILE COVERS 1907 - 1 Mar 2007 VOL 146 ISS 10
FILE LAST UPDATED: 28 Feb 2007 (20070228/ED)

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=> s l7
L8 73 L7

=> d ibib abs hitstr 50-73

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10526940claim4

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	127.42	572.95

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-18.72	-46.80

FILE 'REGISTRY' ENTERED AT 17:21:58 ON 01 MAR 2007
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STRUCTURE FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1
DICTIONARY FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10526940last.str

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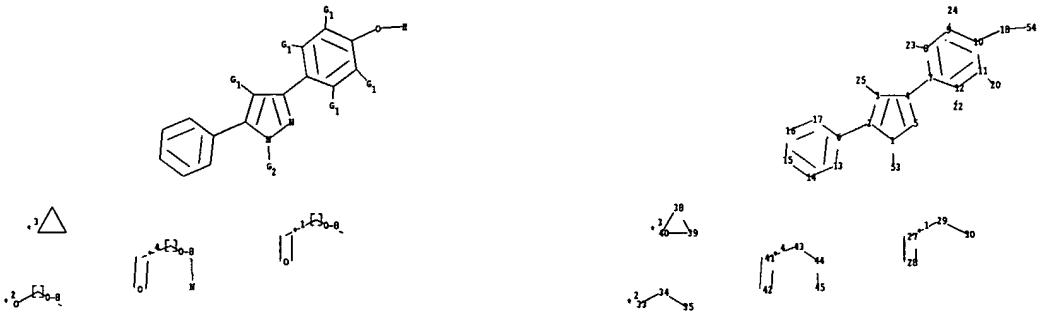
10526940claim4



chain nodes :
18 20 22 23 24 25 27 28 29 30 33 34 35 41 42 43 44 45 53 54
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 38 39 40
chain bonds :
1-53 2-6 3-25 4-7 8-23 9-24 10-18 11-20 12-22 18-54 27-29 27-28 29-30
33-34 34-35 41-42 41-43 43-44 44-45
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14
14-15 15-16 16-17 38-39 38-40 39-40
exact/norm bonds :
1-2 1-5 1-53 3-25 4-5 8-23 9-24 10-18 11-20 12-22 27-28 33-34 41-42
44-45
exact bonds :
2-3 2-6 3-4 4-7 18-54 27-29 29-30 34-35 38-39 38-40 39-40 41-43 43-44
normalized bonds :
6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 6 : 7 : 38 :

G1:H,CH3

G2:H,Ak,[*1],[*2],[*3],[*4]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
33:CLASS 34:CLASS 35:CLASS 38:Atom 39:Atom 40:Atom 41:CLASS 42:CLASS
43:CLASS 44:CLASS 45:CLASS 53:CLASS 54:CLASS

Karen Cheng

10526940claim4

```
L9      STRUCTURE UPLOADED

=> d
L9 HAS NO ANSWERS
L9              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> d his

     (FILE 'HOME' ENTERED AT 17:14:23 ON 01 MAR 2007)

     FILE 'REGISTRY' ENTERED AT 17:14:32 ON 01 MAR 2007
L1              STRUCTURE UPLOADED
L2           854 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 17:14:57 ON 01 MAR 2007
L3           155 S L2

     FILE 'REGISTRY' ENTERED AT 17:16:13 ON 01 MAR 2007
L4              STRUCTURE UPLOADED
L5           671 S L4 FULL  SUB=L2

     FILE 'STNGUIDE' ENTERED AT 17:16:48 ON 01 MAR 2007

     FILE 'REGISTRY' ENTERED AT 17:20:20 ON 01 MAR 2007
L6              STRUCTURE UPLOADED
L7           165 S L6 FULL  SUB=L2

     FILE 'CAPLUS' ENTERED AT 17:20:51 ON 01 MAR 2007
L8            73 S L7

     FILE 'REGISTRY' ENTERED AT 17:21:58 ON 01 MAR 2007
L9              STRUCTURE UPLOADED

=> s l9 full sub=l7
FULL SUBSET SEARCH INITIATED 17:22:31 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -      165 TO ITERATE

100.0% PROCESSED      165 ITERATIONS                          100 ANSWERS
SEARCH TIME: 00.00.01

L10          100 SEA SUB=L7 SSS FUL L9

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                41.10     614.05
```

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10526940claim4

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-46.80

FILE 'CAPLUS' ENTERED AT 17:22:34 ON 01 MAR 2007
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FILE COVERS 1907 - 1 Mar 2007 VOL 146 ISS 10
FILE LAST UPDATED: 28 Feb 2007 (20070228/ED)

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They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l10
L11 13 L10

=> d ibib abs hitstr tot

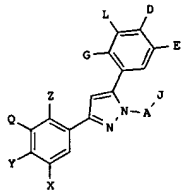
Karen Cheng

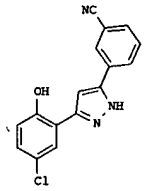
L11 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1095978 CAPLUS
DOCUMENT NUMBER: 145:438611
TITLE: Preparation of 3,5-diphenylpyrazoles as antitumor agents
INVENTOR(S): Kuroiwa, Shunsuke; Maruyama, Sakiko; Suzuki, Yoshikazu; Yamazaki, Hiroko
PATENT ASSIGNEE(S): Nippon Kayaku Kabushiki Kaisha, Japan
SOURCE: PCT Int. Appl., 45pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006109680	A1	20061019	WO 2006-JP307346	20060406

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

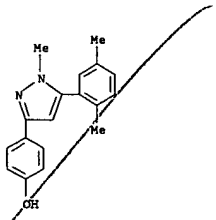
PRIORITY APPLN. INFO.: JP 2005-110717 A 20050407
OTHER SOURCE(S): MARPAT 145:438611
GI


I


II

AB Title compds. I [wherein A = H, carbonyl or sulfonyl; J = (un)substituted alkyl or amino; G, Z = H, OH, alkoxy, etc.; D, E, L, Q, X, Y = H,

L11 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(un)substituted aminocarbonyl, alkoxycarbonyl, etc., D and L, and Q and Y may link together to form a N/S-heterocyclyl ring, with limitations] and pharmaceutically acceptable salts thereof were prepd. as anticancer agents. For instance, treatment of 5'-chloro-2'-hydroxyacetophenone with 3-cyanobenzoyl chloride followed by cyclization with hydrazine hydrate gave diphenylpyrazole II. This product showed cell growth inhibition with IC50 of 0.23 μg/mL against MCF-7 cells and 0.066 μg/mL against MDA-MB-453 cells, resp. Therefore, the invented compds. and their pharmaceutical compns. are useful for the treatment of various cancer, such as breast cancer and lung cancer.
IT 362006-35-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(reference; preparation of diphenylpyrazoles as antitumor agents)
RN 362006-35-7 CAPLUS
CN Phenol, 4-[5-(2,5-dimethylphenyl)-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

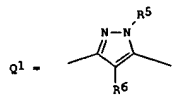


REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1089202 CAPLUS
DOCUMENT NUMBER: 145:439502
TITLE: Epoxy resin compositions, their epoxides having low melting point, and prepregs therewith
INVENTOR(S): Inoue, Kazuya; Hibino, Hiroaki
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 22pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006282531	A	20061019	JP 2005-101698	20050331

PRIORITY APPLN. INFO.: JP 2005-101698 20050331
GI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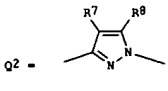
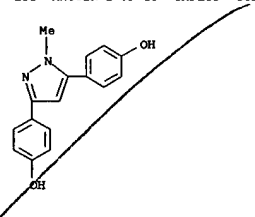

Q2 =

AB The epoxides are GZ-p-C6H2R1R2Y-p-C6H2R3R4ZG [G = glycidyl; R1-R4 = H, halo, C1-8 alkyl(oxy), CN, NO2; Y = Q1, Q2 (R5 = H, C1-8 alkyl; R6-R8 = H, C1-8 alkyl, halo, CN, NO2; Z = single bond, O, C1-8 alkylene)]. Thus, 5 g 4-methoxyacetophenone was reacted with 5.5 g Me 4-methoxybenzoate to give 1,3-bis(4-methoxyphenyl)propane-1,3-dione in 83% yield, which was reacted with methylhydrazine, hydrolyzed, and reacted with epichlorohydrin in the presence of tetrabutylammonium bromide to give 3,5-bis[4-(oxiranylmethoxy)phenyl]-1-methylpyrazole (I; m.p. 127°) in 91% yield. Then, I was reacted with diaminodiphenylmethane, poured in a mold, and kept at 145-155° and then at 180° to give a cured resin.
IT 912804-13-8P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(pyrazolyl group-containing epoxy compds. and their compns. for forming prepregs)
RN 912804-13-8 CAPLUS
CN Phenol, 4,4'-(1-methyl-1H-pyrazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L11 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



Karen Cheng

10526940claim4

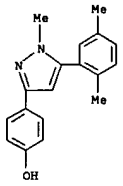
L11 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:211991 CAPLUS
DOCUMENT NUMBER: 140:264528
TITLE: NR3B1 nuclear receptor-binding 3-substituted pyrazole derivatives, and therapeutic uses
INVENTOR(S): Deuschle, Ulrich; Heck, Stefanie; Kober, Ingo; Bauer, Ulrike; Balogh, Imola
PATENT ASSIGNEE(S): Lion Bioscience A.-G., Germany
SOURCE: Eur. Pat. Appl., 45 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1398029	A1	20040317	EP 2002-20256	20020910
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
WO 2004024148	A1	20040325	WO 2003-EP7066	20030702
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003250877	A1	20040430	AU 2003-250877	20030702
US 2006148876	A1	20060706	US 2005-526940	20051021
PRIORITY APPLN. INFO.:			EP 2002-20256	A 20020910
			WO 2003-EP7066	W 20030702

current app.

OTHER SOURCE(S): MARPAT 140:264528
AB The invention discloses pyrazole derivs. which bind to the NR3B1 receptor and act as antagonists of the NR3B1 receptor. The invention further relates to the treatment of diseases and/or conditions through binding of the nuclear receptor by the compds., as well as the production of medicaments using the compds.
IT 362006-35-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(NR3B1 nuclear receptor-binding pyrazole derivs., and therapeutic uses)
RN 362006-35-7 CAPLUS
CN Phenol, 4-[5-(2,5-dimethylphenyl)-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L11 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



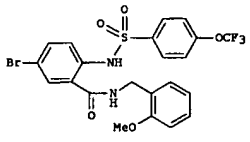
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

102E

L11 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:551386 CAPLUS
DOCUMENT NUMBER: 139:117209
TITLE: Preparation of biaryl phosphate transport inhibitors
INVENTOR(S): Jozefiak, Thomas H.; Bastos, Cecilia M.; Papoulis, Andrew T.; Holmes-Farley, Stephen Randall
PATENT ASSIGNEE(S): Genzyme Corporation, USA
SOURCE: PCT Int. Appl., 135 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003057225	A2	20030717	WO 2002-US41481	20021224
WO 2003057225	A3	20040408		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004019113	A1	20040129	US 2002-327627	20021220
US 7119120	B2	20061010		
AU 2002367396	A1	20030724	AU 2002-367396	20021224
EP 1465638	A2	20041013	EP 2002-806234	20021224
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005514413	T	20050519	JP 2003-557583	20021224
US 2007021509	A1	20070125	US 2006-489286	20060719
PRIORITY APPLN. INFO.:			US 2001-344660P	P 20011226
			US 2002-371649P	P 20020410
			US 2002-327627	A1 20021220
			WO 2002-US41481	W 20021224

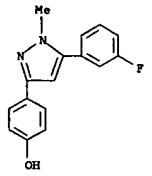
OTHER SOURCE(S): MARPAT 139:117209
GI



II

AB Disclosed are compds. Ar1-W-X-Y-Ar2 [Ar1-2 = (un)substituted aryl group or 5-6 membered non-aromatic group fused to a (un)substituted monocyclic aryl group; W, Y = covalent bond, alkylene; X = SO2, SO2-alkyl, SO2-amino, etc; I] which are inhibitors of phosphate transport. For instance,

L11 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
5-bromo-2-[[(4-trifluoromethoxyphenyl)sulfonyl]amino]benzoic acid (prepn. given) is converted to the acid chloride (SOCl2, reflux) and used to acylate 2-methoxybenzyl amine (THF) to give II. Example compds. inhibit phosphate transport in rabbit intestinal brush border membrane vesicles; a select group of example compds. has IC50 = 0-50 μM. I are used to treat a disease assocd. with hyperphosphatemia, as well as a disease mediated by phosphate-transport function.
IT 362016-88-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of biaryl phosphate transport inhibitors)
RN 362016-88-4 CAPLUS
CN Phenol, 4-[5-(3-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



eg. 44.

eg. 47 = 103.

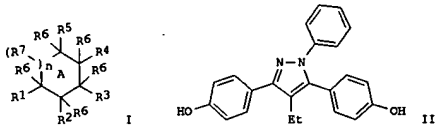
Karen Cheng

10526940claim4

L11 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:240935 CAPLUS
DOCUMENT NUMBER: 132:279214
TITLE: Preparation of non-steroidal estrogen receptor subtype-selective ligands
INVENTOR(S): Katzenellenbogen, John A.; Katzenellenbogen, Benita S.; Fink, Brian E.; Stauffer, Shaun R.; Mortensen, Deborah S.; Sattigeri, Viswajanani Jitendra; Huang, Ying
PATENT ASSIGNEE(S): Board of Trustees of the University of Illinois, USA
SOURCE: PCT Int. Appl., 134 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

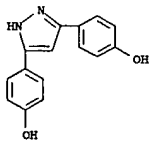
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000019994	A1	20000413	WO 1999-US22747	19991001
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 1998-102881P P 19981002
OTHER SOURCE(S): MARPAT 132:279214
GI

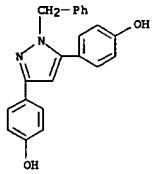


AB Ph substituted pyrazoles, cyclopentadienes, furans, pyrimidines, and their analogs (I) [wherein x = 0 or 1; when x = 0, A = doubly unsatd. 5-membered ring; when x = 1, A = aromatic 6-membered ring; R1 = (un)substituted Ph; R2-R5 and R7 = independently H, basic or polar group, or (un)substituted Ph, alkyl, alkenyl, or alkynyl; or R7 is not present; R6 = H, basic or polar group, or (un)substituted alkyl, alkenyl, alkynyl, or alkoxy; or R6 is not present] were prepared for selective regulation of cellular activity under the control of estrogen receptor (ER) and for the treatment of

L11 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
hormone-dependent disorders, such as hormone-responsive breast cancer. I have modular structures, which are amenable to solid phase synthesis and the application of combinatorial synthetic methods (no data). I exhibit a spectrum of selective affinities for ERα and ERβ and a spectrum of agonist/antagonist properties. For example, 2-ethyl-1,3-bis(4-methoxyphenyl)-1,3-propanedione was treated with Ph hydrazine.HCl in DMF/THF (89%), followed by BBr3 demethylation in CH2Cl2 to give II (54%). The latter displayed a relatively high ER binding affinity (RBA = 14.0). II also proved to be an ERα potency selective agonist compared to estradiol and showed a 120-fold higher potency in activating transcription via ERα than via ERβ.
IT 137646-99-2P, 3,5-Di(4-hydroxyphenyl)-1H-pyrazole
234093-03-9P, 1-Benzyl-3,5-di(4-hydroxyphenyl)-1H-pyrazole
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of non-steroidal estrogen receptor subtype-selective ligands)
RN 137646-99-2 CAPLUS
CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)



RN 234093-03-9 CAPLUS
CN Phenol, 4,4'-[1-(phenylmethyl)-1H-pyrazole-3,5-diyl]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

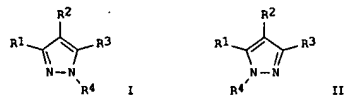
L11 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L11 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:117030 CAPLUS
DOCUMENT NUMBER: 132:166234
TITLE: Preparation of estrogen receptor modulating pyrazoles
INVENTOR(S): Huebner, Verena D.; Lin, Xiaodong; James, Ian; Chen, Liya; Desai, Manoj; Krywult, Beata; Singh, Rajinder; Wang, Liang
PATENT ASSIGNEE(S): Chiron Corp., USA
SOURCE: PCT Int. Appl., 124 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000007996	A2	19990806	WO 1999-US17799	19990806
WO 2000007996	A3	20000831		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9954677	A1	20000228	AU 1999-54677	19990806
EP 1102753	A2	20010530	EP 1999-940917	19990806
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6291505	B1	20010918	US 1999-369747	19990806
JP 2002522422	T	20020723	JP 2000-563630	19990806
US 2002111374	A1	20020815	US 2001-954039	20010918
US 2004034081	A9	20040219		
US 6727273	B2	20040427		
US 2004077701	A1	20040422	US 2003-461914	20030612

PRIORITY APPLN. INFO.: US 1998-95772P P 19980807
US 1998-95773P P 19980807
US 1999-369747 A3 19990806
WO 1999-US17799 W 19990806
US 2001-954039 A1 20010918

OTHER SOURCE(S): MARPAT 132:166234
GI



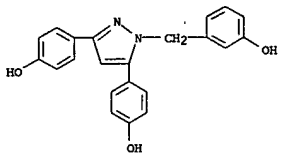
AB The title compds. [I and II; R1, R3 = alkyl, aryl, heteroaryl, etc.; R2 = H, halo, CN, etc.; R4 = H, CO2H, CHO, etc.] which have been found to have unexpected and surprising activity in modulating estrogen receptor activity, and therefore are useful for treating or preventing estrogen

Karen Cheng

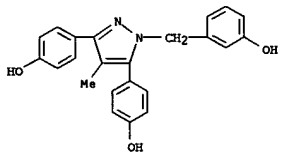
L11 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
receptor-mediated disorders such as osteoporosis, breast and endometrial cancers, atherosclerosis, and Alzheimer's disease, were prepd. E.g., a multi-step synthesis of II [R1 = Ph2CH; R2 = Et; R3 = 4-HOC6H4; R4 = Me], starting with 4'-methoxybutyrylphenone and 2,2-diphenylacetyl chloride, was given (no data for intermediates). Biol. data for compds. I and II were presented.

IT 258847-24-4P 258847-27-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of estrogen receptor modulating pyrazoles)

RN 258847-24-4 CAPLUS
CN Phenol, 3-[[3,5-bis(4-hydroxyphenyl)-1H-pyrazol-1-yl]methyl]- (9CI) (CA INDEX NAME)

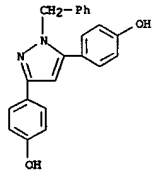


RN 258847-27-7 CAPLUS
CN Phenol, 3-[[3,5-bis(4-hydroxyphenyl)-4-methyl-1H-pyrazol-1-yl]methyl]- (9CI) (CA INDEX NAME)

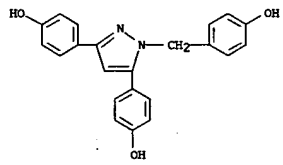


L11 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CN Phenol, 4,4'-[1-(phenylmethyl)-1H-pyrazole-3,5-diyl]bis- (9CI) (CA INDEX NAME)



RN 234093-04-0 CAPLUS
CN Phenol, 4,4'-[1-[(4-hydroxyphenyl)methyl]-1H-pyrazol-3,5-diyl]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

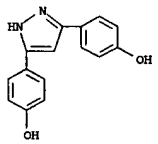
L11 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:327909 CAPLUS
DOCUMENT NUMBER: 131:125589
TITLE: Novel structural templates for estrogen-receptor ligands and prospects for combinatorial synthesis of estrogens
AUTHOR(S): Fink, Brian E.; Mortensen, Deborah S.; Stauffer, Shaun R.; Aron, Zachary D.; Katzenellenbogen, John A.
CORPORATE SOURCE: Department of Chemistry, University of Illinois, Urbana, IL, 61801, USA
SOURCE: Chemistry & Biology (1999), 6(4), 205-219
CODEN: CBOLE2; ISSN: 1074-5521
PUBLISHER: Current Biology Publications
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The development of estrogen pharmaceutical agents with appropriate tissue-selectivity profiles has not yet benefited substantially from the application of combinatorial synthetic approaches to the preparation of structural classes that are known to be ligands for the estrogen receptor (ER). We have developed an estrogen pharmacophore that consists of a simple heterocyclic core scaffold, amenable to construction by combinatorial methods, onto which are appended 3-4 peripheral substituents that embody substructural motifs commonly found in nonsteroidal estrogens. The issue addressed here is whether these heterocyclic core structures can be used to prepare ligands with good affinity for the ER. We prepared representative members of various azole core structures. Although members of the imidazole, thiazole or isoxazole classes generally have weak binding for the ER, several members of the pyrazole class show good binding affinity. The high-affinity pyrazoles bear close conformational relationship to the nonsteroidal ligand raloxifene, and they can be fitted into the ligand-binding pocket of the ER-raloxifene X-ray structure. Compds. such as these pyrazoles, which are novel ER ligands, are well suited for combinatorial synthesis using solid-phase methods.

IT 137646-99-2P 234093-03-9P 234093-04-0P
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(azoles as structural templates for estrogen-receptor ligands and prospects for combinatorial synthesis of estrogens)

RN 137646-99-2 CAPLUS
CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)



RN 234093-03-9 CAPLUS

L11 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

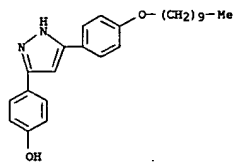
ACCESSION NUMBER: 1997:86817 CAPLUS
DOCUMENT NUMBER: 126:179299
TITLE: FLCs with a five-membered ring in the mesogenic core
AUTHOR(S): Iglesias, R.; Serrano, J. L.; Sierra, T.
CORPORATE SOURCE: Fac. Cienc.-Inst. Cienc. Mater. Aragon, Univ. Zaragoza, Zaragoza, 50009, Spain
SOURCE: Liquid Crystals (1997), 22(1), 37-46
CODEN: LICRE6; ISSN: 0267-8292
PUBLISHER: Taylor & Francis
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A study was undertaken of the structure-activity relation of eight new chiral compds. having either a pyrazole or an isoxazole ring as a central bridge in the mesogenic core. The presence of dimers in the pyrazole compds. accounts for their lower Ps values in comparison with the isoxazole analogs. The corresponding four β-diketone precursors also were studied and these, as expected given their bent mol. shape, show much worse mesomorphic and ferroelec. behavior. To complete the study, the mol. dipoles of the three types of derivative were determined using AM1 calcns.

Two types of chiral tail were incorporated into the compds.: alkoxy and alkanoyloxy. The latter tail gives rise to the best mesomorphic and ferroelec. properties. A study of the tail conformation by MM2 calcns. provides an explanation of these results. The highest Ps value (137 nC cm-2) was obtained for the isoxazole derivative with the (2S)-2-butyloxypropanoyloxy chiral tail. The potential of all twelve compds. as chiral dopants for FLC mixts. was evaluated by a study of 10 mol.% binary mixts. in a standard host system.

IT 187334-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with Bu lactate)

RN 187334-75-4 CAPLUS
CN Phenol, 4-[5-[4-(decyloxy)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



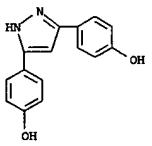
10526940claim4

L11 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:614968 CAPLUS
DOCUMENT NUMBER: 125:248658
TITLE: Synthesis and properties of poly(arylene ether pyrazole)s
AUTHOR(S): Srinivasan, K. R.; Bass, R. G.; Smith, J. G.
CORPORATE SOURCE: Dep. Chem., Virginia Commonwealth Univ., Richmond, VA, 23284-2006, USA
SOURCE: High Performance Polymers (1996), 8(3), 381-393
CODEN: HPPOEX; ISSN: 0954-0083
PUBLISHER: Institute of Physics Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Poly(arylene ether pyrazole)s containing NH and NPh groups were prepared by the aromatic nucleophilic displacement reaction of two new bisphenols containing a pyrazole ring with activated aromatic dihalides in N,N-dimethylacetamide at 155° in the presence of anhydrous potassium carbonate. The polymers exhibited glass transition temps. (Tg) ranging from 190-296° and inherent viscosities from 0.44-1.96 dL g-1. Poly(arylene ether-pyrazole)s containing NH groups exhibited higher Tg and mech. properties than the corresponding N-phenyl-containing poly(arylene ether pyrazole)s. The chemical, phys. and mech. properties of these polymers are discussed.

IT 137646-99-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(monomer; for synthesis of bis(hydroxyphenyl)pyrazoles)

RN 137646-99-2 CAPLUS
CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)



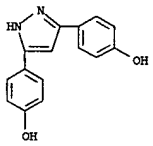
IT 137647-00-8P 137647-01-9P 137661-49-5P
182233-43-8P 182233-58-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and properties of poly(arylene ether pyrazoles))

RN 137647-00-8 CAPLUS
CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis-, polymer with 1,1'-sulfonylbis[4-chlorobenzene] (9CI) (CA INDEX NAME)

CM 1

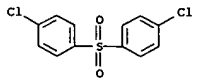
CRN 137646-99-2

L11 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C15 H12 N2 O2



CM 2

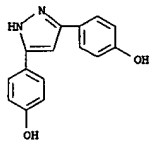
CRN 80-07-9
CMF C12 H8 Cl2 O2 S



RN 137647-01-9 CAPLUS
CN Methanone, 1,3-phenylenebis[(4-chlorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)

CM 1

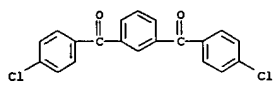
CRN 137646-99-2
CMF C15 H12 N2 O2



CM 2

CRN 22198-44-3

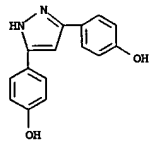
L11 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C20 H12 Cl2 O2



RN 137661-49-5 CAPLUS
CN Methanone, bis(4-chlorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)

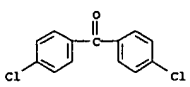
CM 1

CRN 137646-99-2
CMF C15 H12 N2 O2



CM 2

CRN 90-98-2
CMF C13 H8 Cl2 O

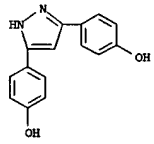


RN 182233-43-8 CAPLUS
CN Methanone, 1,4-phenylenebis[(4-fluorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)

CM 1

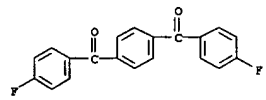
CRN 137646-99-2
CMF C15 H12 N2 O2

L11 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

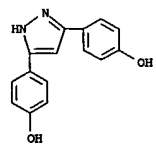
CRN 68418-51-9
CMF C20 H12 F2 O2



RN 182233-58-5 CAPLUS
CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis-, polymer with bis(4-fluorophenyl)phenylphosphine oxide (9CI) (CA INDEX NAME)

CM 1

CRN 137646-99-2
CMF C15 H12 N2 O2

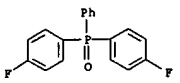


CM 2

CRN 54300-32-2
CMF C18 H13 F2 O P

Karen Cheng

L11 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



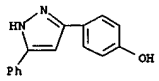
L11 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:639383 CAPLUS
DOCUMENT NUMBER: 121:239383
TITLE: Stability constants of iron(III), chromium(III) and aluminum(III) chelates with some substituted pyrazoles
AUTHOR(S): Sawalakhe, P. D.; Narwade, M. L.; Wadodkar, K. N.
CORPORATE SOURCE: Department of Chemistry, Vidarbha Mahavidyalaya, Amravati, 444 604, India
SOURCE: Journal of the Indian Chemical Society (1994), 71(1), 49-51
CODEN: JICSAH; ISSN: 0019-4522
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The interactions of Fe3+, Cr3+ and Al3+ metal ions with 3-(2-hydroxyphenyl)-5-phenylpyrazole, 3-(2-hydroxy-5-methylphenyl)-5-phenylpyrazole and 3-(2-hydroxy-5-methylphenyl)-5-(4-methoxyphenyl)pyrazole have been investigated potentiometrically in 70% dioxane-water mixture as a solvent at 0.1 M ionic strength. The proton-ligand and metal-ligand stability consts. were determined

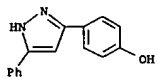
IT 75059-29-9
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(ionization constant of)

RN 75059-29-9 CAPLUS
CN Phenol, 4-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)



IT 75059-29-9D, transition metal complexes
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(stability constant of)

RN 75059-29-9 CAPLUS
CN Phenol, 4-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

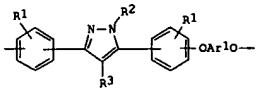


L11 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:135439 CAPLUS
DOCUMENT NUMBER: 120:135439
TITLE: Aromatic polyethers containing pyrazole units and monomers for their preparation
INVENTOR(S): Pfaendner, Rudolf; Wolf, Jean Pierre; Kainmueller, Thomas; Kramer, Andreas; Hoffmann, Kurt; Stockinger, Friedrich
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Ger. Offen., 17 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4230839	A1	19930325	DE 1992-4230839	19920915
PRIORITY APPLN. INFO.:			CH 1991-2753 A	19910918

GI



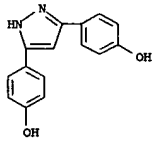
I

AB Polyethers with good thermal stability and solubility in organic solvents contain 1-100 mol% segments I (R1, R3 = alkyl, alkoxy, aryl, aryloxy, halogen; R2 = H, alkyl, Ph; Ar1 = dihalogenated arylene activated for nucleophilic exchange) and 99-0 mol% segments -OAr2OAr1- (Ar2 = arylene). Treatment of Et 4-methoxybenzoate with NaH and then condensation with 4-methoxyacetophenone in glyme gave 68% 1,3-bis(4-methoxyphenyl)-1,3-propanedione, cyclization of which with N2H4.H2O gave 42% 3,5-bis(4-methoxyphenyl)pyrazole, which was demethylated by C5H5N.HCl in 61% yield to the bisphenol (II). Heating II 0.0501, 4,4'-sulfonyldiphenol 0.1562, (4-ClC6H4)2SO2 0.2001, and K2CO3 0.2116 mol for 6 h at 225-280° gave a polyether with reduced viscosity 0.45 dL/g, glass temperature 223°, decomposition temperature (TGA) 510°, and solubility in N-methylpyrrolidone and CH2Cl2 >25%.

IT 137646-99-2P, 4,4'-(3,5-Pyrazolediyl)diphenol
RL: PREP (Preparation)
(preparation of)

RN 137646-99-2 CAPLUS
CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L11 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

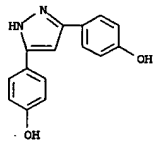


IT 151485-79-9P
RL: PREP (Preparation)
(preparation of heat-resistant, with good solubility)

RN 151485-79-9 CAPLUS
CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis-, polymer with 1,1'-sulfonylbis[4-chlorobenzene] and 4,4'-sulfonylbis[phenol] (9CI) (CA INDEX NAME)

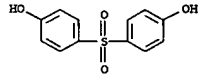
CM 1

CRN 137646-99-2
CMF C15 H12 N2 O2



CM 2

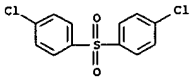
CRN 80-09-1
CMF C12 H10 O4 S



CM 3

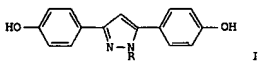
CRN 80-07-9
CMF C12 H8 Cl2 O2 S

L11 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L11 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:680692 CAPLUS
DOCUMENT NUMBER: 115:280692
TITLE: Synthesis of poly(arylene ether pyrazoles) by aromatic nucleophilic displacement reactions
AUTHOR(S): Bass, R. G.; Srinivasan, K. R.
CORPORATE SOURCE: Dep. Chem., Virginia Commonw. Univ., Richmond, VA, 23284-2006, USA
SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1991), 32(1), 619-20
CODEN: ACPPAY; ISSN: 0032-3934
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Title polyethers were prepared by the condensation of bisphenols I (R = H, Ph) with dihalides 4-R1C6H4XC6H4R1-4 (R1 = Cl, F; X = CO, SO2, isophthaloyl, terephthaloyl, 4-COC6H4OC6H4CO-4).

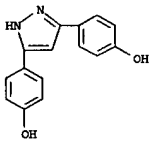
IT 137647-00-8P 137647-01-9P 137647-02-0P
137661-49-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and properties of)

RN 137647-00-8 CAPLUS

CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis-, polymer with 1,1'-sulfonylbis[4-chlorobenzene] (9CI) (CA INDEX NAME)

CM 1

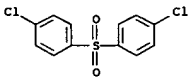
CRN 137646-99-2
CMF C15 H12 N2 O2



CM 2

L11 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 80-07-9
CMF C12 H8 Cl2 O2 S

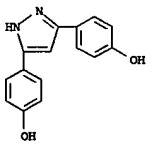


RN 137647-01-9 CAPLUS

CN Methanone, 1,3-phenylenebis[(4-chlorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)

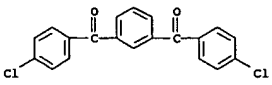
CM 1

CRN 137646-99-2
CMF C15 H12 N2 O2



CM 2

CRN 22198-44-3
CMF C20 H12 Cl2 O2



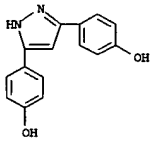
RN 137647-02-0 CAPLUS

CN Methanone, 1,4-phenylenebis[(4-chlorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)

CM 1

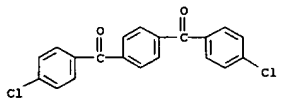
CRN 137646-99-2
CMF C15 H12 N2 O2

L11 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 22198-42-1
CMF C20 H12 Cl2 O2

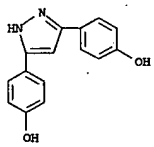


RN 137661-49-5 CAPLUS

CN Methanone, bis(4-chlorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)

CM 1

CRN 137646-99-2
CMF C15 H12 N2 O2

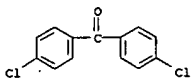


CM 2

CRN 90-98-2
CMF C13 H8 Cl2 O

Karen Cheng

L11 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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ACCESSION NUMBER: 1980:567052 CAPLUS
DOCUMENT NUMBER: 93:167052
TITLE: Luminescence properties of arylpyrazoles
AUTHOR(S): Udachin, Yu. M.; Chursinova, L. V.; Przheval'skii, N. M.; Grandberg, I. I.; Tokmakov, G. P.
CORPORATE SOURCE: Mosk. S-kh. Akad., Moscow, USSR
SOURCE: Izvestiya Timiryazevskoi Sel'skokhozyaistvennoi Akademii (1980), (3), 162-9
CODEN: ITSAA7; ISSN: 0021-342X
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The absorption and emission spectra and luminescence quantum yields of mono-, di-, and triarylpyrazoles were determined in different solvents and at
liquid N and room temperature Steric effects played a major role, e.g., 1,5-diarylpyrazoles exhibited absorption maximum at shorter wavelengths than 1,3- or 1,4-diarylpyrazoles owing to aryl ring interaction, which decreased the coplanarity of the mol. Triarylpyrazoles showed severe fluorescence quenching for the same reason. Calcn. of the charge distribution in the ground (S0) and excited singlet (S1) states of 1,3-diphenylpyrazole indicated that excitation was accompanied by transfer of electron d. from N-1, C-3, and the 3-Ph ring to N-2.

IT 75059-29-9
RL: PRP (Properties)
(absorption and fluorescence spectra of)
RN 75059-29-9 CAPLUS
CN Phenol, 4-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)